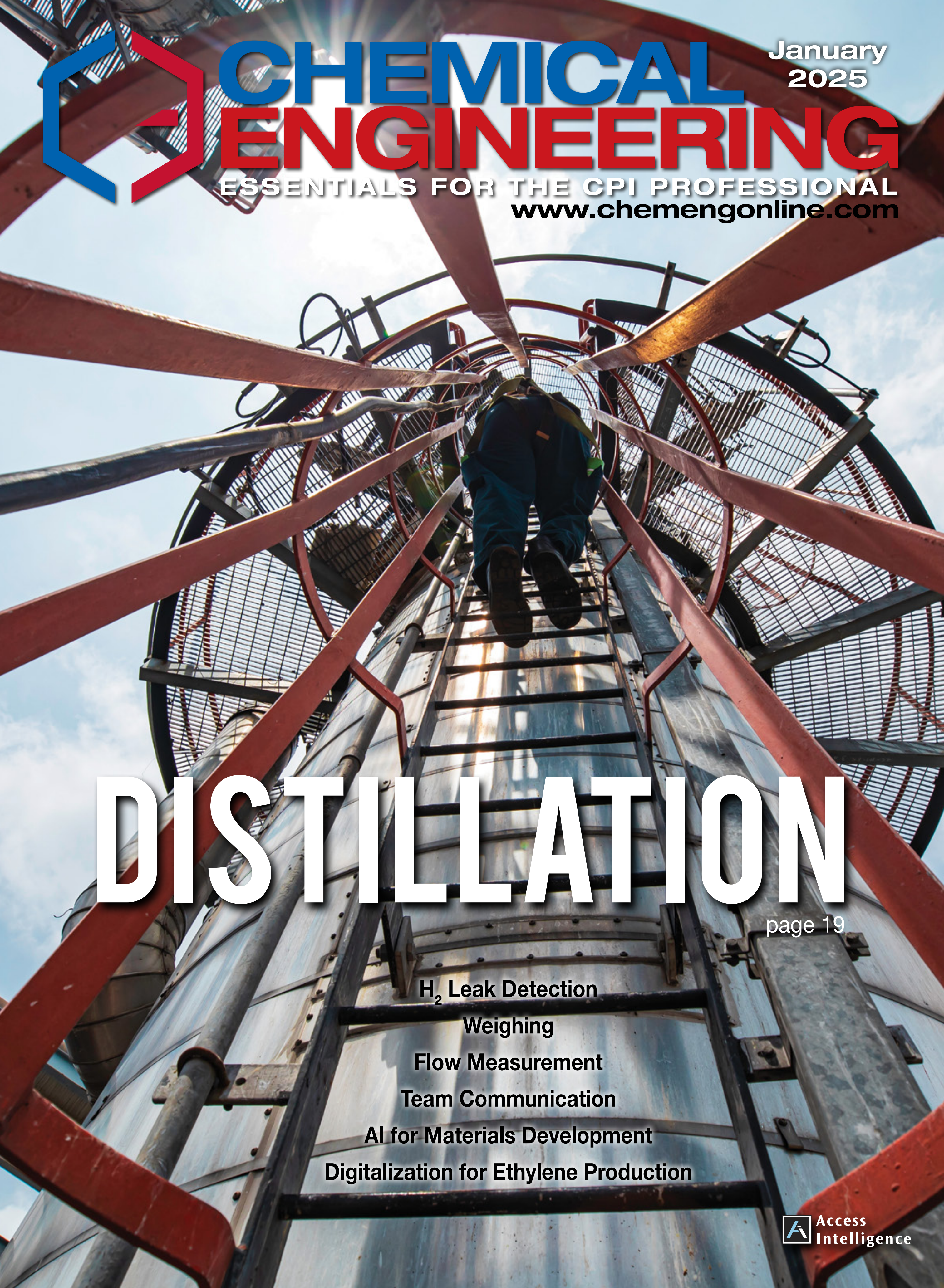

January 2025

# CHEMICAL ENGINEERING

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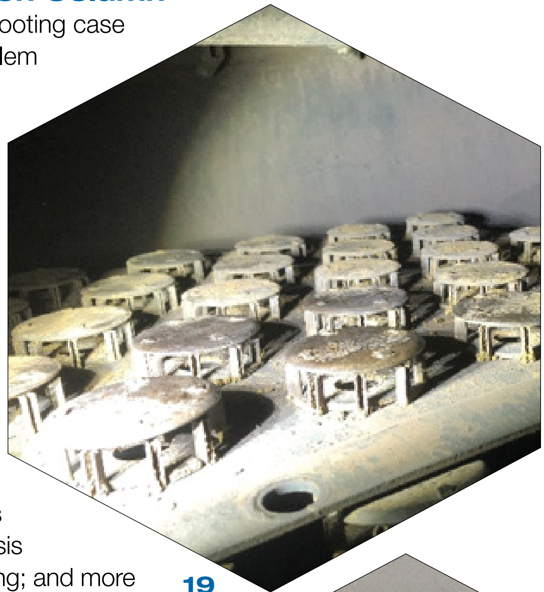

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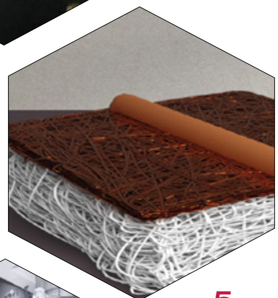

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# Editor's Page

## CPI Outlook for 2025

The industrial sector consumes more than 80% of basic and specialty chemicals. Worldwide, industrial activity saw a modest recovery in 2024. Global industrial production is expected to have increased by 1.3% by the end of 2024, with predictions of about 2.6% growth in 2025. These findings are according to the American Chemistry Council (ACC; Washington, D.C.; americanchemistry.com) [*1*].

The demand for chemicals remained weak in 2024, even though the destocking cycle that resulted from the pandemic-related high inventories from a few years ago has essentially ended. Two important end-use markets for chemistry products are automobiles and housing. An average car in North America contains more than $4,400 of chemistry products, including 426 lb of plastics and composites; and an average single-family home contains about 33,000 lb of chemistry products. Both markets faced challenges in 2024 as the cost for automobile ownership escalated and the housing market struggled. Both are expected to improve in 2025 as interest rates fall in the U.S. [*1*]

### Growth areas

Capital spending rose 4.1% to $34 billion in 2024 and is expected to grow another 2.9% in 2025 [*1*]. Strong growth areas were new investments in chemicals for the semiconductor and electronics industries, battery development and other sustainability-related areas. In the U.S., government funding resulting from legislation, such as the Inflation Reduction Act (IRA), the Creating Helpful Incentives to Produce Semiconductors (CHIPS) and Science Act have driven investments in these sectors.

The semiconductor industry surge is driven by increased demands for computing and data storage (datacenters) and electronics, resulting from increased use of machine learning, artificial intelligence (AI), wireless communication, autonomous driving, electric vehicles and more. The ACC says that manufacture of semiconductors requires about 500 different process chemicals.

In a recent report [*2*], McKinsey Global Institute identified semiconductors, along with batteries, electric vehicles, robotics, biotechnology and 13 other industries with high growth potential, as arenas that have the potential to significantly affect the global economy.

### Looking ahead

In its 2025 Chemical Industry Outlook [*3*], Deloitte highlights five trends that may help industry leaders plan for the coming years, including a look at cost efficiency, end markets, innovation, sustainability and supply chains.

The ACC projects a positive long-term outlook for the U.S. chemical industry. The U.S. continues to maintain a production advantage due to feedstocks from natural gas, and trade remains vital to the industry, which continues to maintain a trade surplus. Risks include uncertainties around geopolitical conflicts, trade disruptions, regulatory impacts and unexpected events, such as from extreme weather. ■

*Dorothy Lozowski, Editorial Director*

1. American Chemistry Council, Chemical Production Steady Amid Weak Recovery in Key End-Use Markets, ACC Year-End Situation & Outlook 2024.
2. McKinsey Global Institute, The Next Big Arenas of Competition, Oct. 23, 2024, www.mckinsey.com/mgi/our-research/the-next-big-arenas-of-competition.
3. Deloitte Research Center for Energy & Industrials, 2025 Chemical Industry Outlook, Nov. 4, 2024, www2.deloitte.com/us/en/insights/industry/oil-and-gas/chemical-industry-outlook.html.

## Electrically powered heat pumps and vacuum pumps simplify $CO_2$-capture retrofits

Meeting climate-change goals requires steep reductions in greenhouse-gas emissions from existing power plants and hard-to-abate industry operations. However, the energy required to release captured $CO_2$ from sorbent material is a challenge for the economic viability of these efforts. Also, retrofitting carbon-capture and storage (CCS) systems onto existing plants can be complicated and costly. Now, a CCS technology using electrically driven heat and vacuum pumps is positioned to address both issues, especially in situations where little or no waste heat is available from the host plant.

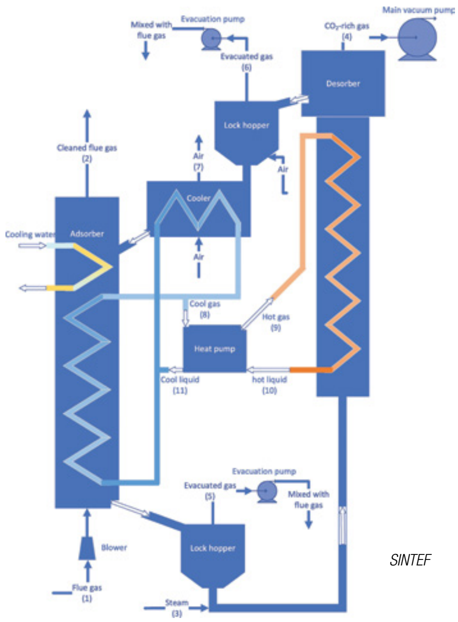
The technology, known as continuous swing adsorption reactor (CSAR), was developed by researchers at the independent research organization SINTEF (Trondheim, Norway; www.sintef.no), along with collaborators at CCS technology developer Caox AS (Stavanger, Norway; www.caox.no). A successful demonstration using CSAR to capture $CO_2$ from fluegas was recently completed at a waste incineration facility near Bergen, Norway. CSAR represents a novel approach to providing heat for releasing $CO_2$ from sorbent material, and can be cost-effectively retrofitted onto existing facilities because it is powered by electricity rather than steam.

CSAR features two fluidized-bed reactors (diagram), one for adsorbing $CO_2$ from fluegas, and the other for desorption of the gas. As the fluegas enters the first reactor, the $CO_2$ is adsorbed by polyethyleneimine (PEI) sorbent, which circulates between the two reactors. "This binding process occurs at low temperature and generates heat," says Jan Hendrik Cloete, SINTEF research scientist. The heat is then transferred to the desorption reactor via a heat pump, where it is used to release the $CO_2$ from the sorbent, this time at a higher temperature. "The heat pump is used to transfer the heat between the reactors, while the vacuum pump assists in releasing the $CO_2$," he explains.

Combined, the two pumps transfer heat efficiently, and consume minimal energy. Because both pumps use conventional electricity, installation on existing plants is straightforward.

The research showed that "CSAR technology competes very well with other [CCS] technologies that utilize heat" [such as temperature-swing adsorption], says Cloete. "This applies in particular if reasonably priced electricity from renewable sources is available," he says.

Following the successful demonstration at the waste incinerator, SINTEF plans to further test the 100-kg-per-day $CO_2$ pilot plant at a cement factory in Spain in 2026.




SINTEF

## Single-atom catalysis reduces water-splitting costs

One of the main limiting factors in the production of "green" hydrogen via electrochemical water splitting is the relatively slow rate of the oxygen evolution reaction (OER) and the use of very expensive noble metals like iridium to catalyze the reaction. Now, a team of scientists from University of Bayreuth in Germany (www.uni-bayreuth.de) and Shenzhen University in China (en.szu.edu.cn), led by professor Francesco Ciucci, have demonstrated a novel atomic geometry to catalyze the reaction, significantly improving OER activity while also reducing the volume of noble metals used. Their method disperses individual iridium atoms — in a much smaller amount than typically required for OER — coupled with dimethylimidazole (MI) and cobalt-iron (CoFe) hydroxide supports, in an out-of-plane orientation.

Another benefit of this method is the ultra-low overpotential (the additional energy required to speed up the reaction) for this catalyst geometry when compared with traditional OER catalysts. Scientists have been studying single-atom catalysis with out-of-plane coordination to improve different electrochemical processes, but this was the first work to report on noble-metal single atoms on metal hydroxides in the context of OER.

The team's work indicated the unique coordination between the single iridium atoms and MI, which they believe redistributes charge around the Ir site and reduces the reaction energy barrier. According to the team, the catalyst synthesis takes place in a simple, two-step process at ambient temperatures and pressures. They also used this method to synthesize additional types of atomically dispersed single-atom geometries supported by porous hydroxide materials, showing that this preparation platform can be used for a wide range of catalytic reactions, including those requiring platinum, palladium and ruthenium.

The researchers have tested the iridium-CoFe-OH-MI catalyst in a two-electrode water-splitting cell in the laboratory, as well as in an anion-exchange membrane (AEM) electrolyzer. In the AEM demonstration, the electrolyzer exhibited stable operation for over 150 h with little degradation at a voltage of 500 $mA\,cm^{-2}$. This work was first described in the October 2024 issue of *Nature Nanotechnology*.

## New electrode design improves electrochemical $CO_2$-to-ethylene conversion

Electrochemically converting carbon dioxide into useful chemicals or fuels is a promising $CO_2$-utilization strategy, but scaling up the process is a challenge. One reason is that the gas-diffusion electrodes (GDEs) used to facilitate contact between gaseous $CO_2$, solid catalyst and liquid electrolyte need to have gas-diffusion layers that are simultaneously hydrophobic and electrically conductive, leading to a tradeoff. Now, researchers at the Massachusetts Institute of Technology (MIT; Cambridge, Mass.; www.mit.edu) have developed a way to get around this tradeoff when designing larger electrodes for scaled-up systems.

Within a GDE, the gas-diffusion layer (GDL) must fulfill three functions, the researchers say: (1) physically support the catalyst, yet be sufficiently porous for gas transport; (2) have adequate electronic conductivity to facilitate electron transport to the catalyst layer with minimal ohmic [resistance] loss; and (3) maintain robust hydrophobicity to ensure that the triple-phase contact is sustained close to the catalyst.

This sets up a tradeoff because highly conductive materials are generally hydrophilic, and the most hydrophobic materials are non-conductive. The MIT team, led by Kripa Varanasi, developed a GDL that achieves both conductivity and hydrophobicity by introducing micro-scale copper conductors that span the hydrophobic membrane (which is made from expanded polytetrafluoroethylene (ePTFE)). Weaving the copper wire through the ePTFE layer provides a highway for electrons to pass with minimal resistance.


The design of the new electrode, which the researchers call a hierarchically conductive GDE platform (photo), eliminates resistance losses that affect conventional ePTFE electrodes, and enable low voltages and high charge-transfer efficiencies for $CO_2$-to-ethylene conversion at pilot scale, the researchers say.

"The improvement of conductivity is achieved with a minimal footprint (<2% area) and without sacrificing the bulk hydrophobicity of the ePTFE," the MIT team writes in a recent issue of *Nature Communications*. The hierarchically conductive GDE approach decouples the electron conduction and hydrophobicity requirements of the GDL, the researchers say, which "unlocks electrode architecture design without placing additional constraints on catalyst or electrolyzer design," and allows the scaleup of GDE-based electrochemical reduction of $CO_2$.

## Rational synthesis techniques lead to improved catalyst for dry methane reforming

Dry reforming of methane (DRM), in which carbon dioxide and methane are combined to form synthesis gas ($H_2$ and CO), is an attractive route to making syngas because it does not require consumption of water and does not produce $CO_2$ like the conventional route, steam-methane reforming. Nickel-based zeolite catalysts can facilitate DRM, but they are subject to rapid deactivation via sintering and coke formation at the temperatures that would be ideal for the conversion at industrial scale.

To alleviate the problem of catalyst deactivation, researchers at the Oak Ridge National Laboratory (ORNL; Oak Ridge, Tenn.; www.ornl.gov) studied the bonding between the nickel active sites and the catalyst support, as well as how the synthesis method affects the catalyst deactivation. The information they gathered allowed them to devise a synthetic process for the catalyst that led to stronger interactions between the metal active sites and the zeolite support material. These strengthened interactions suppressed coke formation and sintering during the DMR reaction.

"The underlying chemistry of Ni-Si interaction in zeolites for the creation of stable catalytic sites is poorly understood, and thus, catalyst optimization defaults to inefficient trial-and-error," writes the ORNL team, led by Felipe Polo-Garzon and Junyan Zhang. "In this study, we establish a fundamental understanding regarding the impact of catalyst synthesis mechanisms on catalyst properties, and ultimately on catalyst performance for DRM."

The synthesis method involves anchoring highly dispersed Ni sites onto de-aluminated zeolite supports. The ORNL researchers found that "dispersion and Ni-zeolite interaction can be precisely controlled by adjusting the airflow during calcination, allowing for tunable metal dispersion ranging from [Ni] nanoparticles to isolated sites within the framework." The high airflow enhanced the removal of decomposition byproducts, which strengthened the Ni-support interaction, the ORNL team hypothesized.

Using a combination of infrared spectroscopy, X-ray absorption spectroscopy and microscopy allowed the scientists to characterize the dispersion of the synthesized Ni species and their interaction with the support. "Structure-performance correlations demonstrated that the finely tuned synthesis method leads to catalysts with significantly enhanced stability during DRM," the researchers write in a paper recently published in *Nature Communications*.

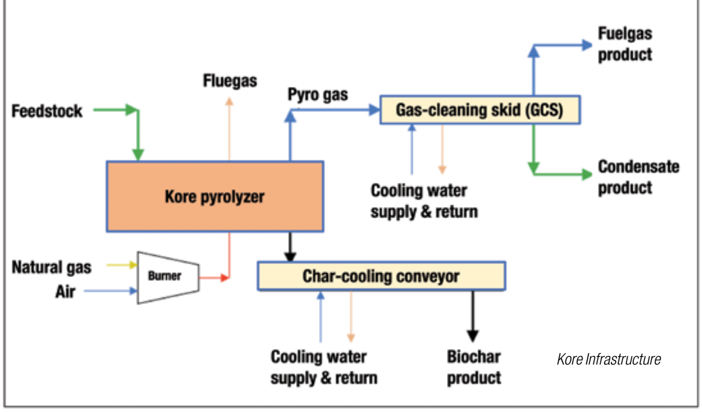
This fundamental understanding of the precision synthesis of active sites and their intrinsic activity opens new avenues to rational catalyst design, the researchers say.

## Oxygen-free slow pyrolysis boosts bio-waste utilization

Biogenic materials, including agricultural residue or other organic waste, hold a considerable amount of energy density in the form of carbon and hydrogen, but efficiently processing these solid materials to harvest energy can pose challenges. The Modular Conversion Technology$^{TM}$ (MCT) developed by Kore Infrastructure (Los Angeles, Calif.; www.koreinfrastructure.com) employs slow pyrolysis in a continuous plug-flow process in the absence of oxygen to convert biomass into a biogas mixture and solid carbon. "We are heating a continuous flow of biogenic feedstocks using slow pyrolysis to upwards of 1,000°F over about 45 to 60 minutes. This combination of temperature plus time volatizes nearly every chemical component except the inorganic ash and fixed carbon," explains Kore senior technical advisor Joe Zuback.

At the beginning of the process (diagram), solid feedstock is reduced in size to around 1-in. in diameter, as needed. It is then fed continuously through two air-lock valves into an upper retort (a large-diameter pipe outfitted with a slow-speed augur to push the feed through). Once the feedstock passes through the first retort, it is dropped into a similar lower retort, exiting again through two air-lock valves that prevent oxygen from entering. Heating gas enters below the lower retort and flows in the interstitial space between retorts in the opposite direction of feedstock flow. "The two horizontal retorts in series are positioned vertically to maximize heat-exchange area in the smallest equipment footprint," mentions Zuback. For the pyrolysis heat source, Kore's process can use combusted gas, stack gas or air heated with waste heat. Heat can also be provided by combustion of a portion of the produced biogas, which could also be used for onsite power generation.

Kore has operated a 1-ton/h pyrolyzer over a two-year period for a project in Los Angeles sponsored by Southern California Natural Gas and the South Coast Air Quality Management District. The company has also begun work to deploy its technology at a landfill operated by Waste Management, Inc. (Houston; www.wm.com) in Lancaster, Calif. to process large solid material leftover from composting operations, as well as demolition wood and other organic waste. "Landfill diversion in California now is being mandated by law, and we think that will expand to other regions. Our MCT is sized small enough to be co-located at a landfill to support the environmental services industry to divert organics and upgrade them for clean energy use, whether it's clean power or hydrogen or renewable natural gas," notes Cornelius Shields, Kore's founder and CEO. Next on the horizon for Kore are installations in the cement industry for producing a renewable coal alternative, and for handling waste in the forestry industry.



Kore Infrastructure

## Confined-channel membrane architecture allows simultaneous oil and water recovery

Surfactants can stabilize oil and water in an emulsion, a useful mechanism in many industrial processes and in cleaning up oil spills. But separating and recovering the oil and water, such as for eliminating waste discharge, can be difficult. A team of researchers from Zhejiang University (Hangzhou, China; www.zju.edu.cn) has developed a membrane system for separating oil and water from complex mixtures that the researchers say can recover up to 97% of water and 75% of oil, both at purities of up to 99.9%.

To achieve this, the team designed a membrane system with narrow, confined channels that can be adjusted between 4 and 125 mm. The channel of membranes — called a Janus channel of membranes, after the two-faced ancient Roman god of transitions and duality — is constructed with pair of hydrophilic and hydrophobic membranes. "The confined Janus channel can amplify the membrane pair through a feedback loop that involves enrichment and demulsification," the researchers, led by Xin-Yu Guo, write in the November 7 issue of *Science*.

As the oil-water emulsion is forced to pass through the narrow channel, pressure drives water to move toward the hydrophilic membrane. This allows water to pass through and results in an elevated concentration of oil within the channel. The increase in oil density triggers hydrodynamic forces that encourage oil droplets to collide and merge, forming larger droplets with reduced surface energy. These larger droplets then pass through the hydrophobic membrane. "This continuous process creates a feedback loop of enrichment, coalescence and demulsification, allowing for the simultaneous, high-purity separation of oil and water without the concentration issues seen in traditional systems," according to a research summary from the American Association for the Advancement of Science (AAAS), publisher of *Science*.

The versatility of the technique "may enable near-zero liquid discharge for a range of separations," the researchers say, such as treatment of oily wastewater and sorting of biological materials. The Janus channel of membranes can process oil-in-water emulsions with oil content as high as 40%, still reaching over 50% water recovery and over 80% oil recovery, the study says.

## Faster kinetics for PFAS removal using existing infrastructure

A next-generation absorbent material with a high affinity for short- and long-chain per- and polyfluoroalkyl substances (PFAS) has recently been granted a patent in the U.S. Developed by Puraffinity Ltd. (London, U.K.; www.puraffinity.com), the material is bottom-up-designed, beginning with a raw substrate, to which functionalized surface coatings are added, explains Puraffinity co-founder and chief product & innovation officer Henrik Hagemann. He emphasizes the significance of using coatings, rather than ligands, for functionalization, which would be much too expensive for large-scale environmental remediation applications. "You can think of the material as a dual-binding adsorbent. There is an electrostatic interaction, and there are hydrophobic and hydrophilic interactions, and this dual-mode interaction basically provides some of the unique benefits," says Hagemann. These benefits include significantly faster kinetics, smaller equipment footprint, longer lifespan and up to 7 times higher PFAS-removal capacity than traditional petroleum-derived ion-exchange resins. "You can run it in 30 or 45 seconds empty bed-contact time, whereas ion-exchange typically needs three to five minutes," he notes.

The material, called Puratech G400, consists of hard, white granules that are around 0.5 mm wide, which are designed to fit into the packed-bed vessels that would typically be used for existing technologies. "We've designed the material's specifications, the actual physical structure of it, to fit into the same paradigm of hydraulic loading and operating conditions as ion-exchange resins, so users can basically keep the same infrastructure," adds Hagemann.

The company has completed extensive third-party validation of its material in several locations across the U.S. and Germany, showing reproducible performance in continuous-flow tests where the absorbent could provide extremely dilute (~4 parts-per-trillion) PFAS concentrations in streams with high (2–8 ppm) total organic content.

Another differentiator is a focus on end-of-life design and material regeneration. Because the favorable kinetics require a smaller material footprint, the waste-disposal volume is reduced, and Puraffinity is preparing to launch a new generation of the material where PFAS can be unbound via liquid-wash next year.

Puraffinity has been working to significantly scale up its synthesis process, and in the last three months, the company has produced over 400 kg of Puratech G400, having recently received U.K. REACH approval for manufacturing at tonnage scale. ■

## Chementator Briefs

### POWERFUL PERMANENT MAGNETS

Permanent magnets — materials that create their own persistent magnetic field — are frequently used in most types of electronics, turbines, engines and motors. Currently, nearly all powerful permanent magnets require rare-earth elements (REEs), such as neodymium or samarium. A new permanent-magnetic material eliminates the need for REEs and their associated environmental and supply-chain risks, instead relying on abundant substances like iron and nitrogen. Through their Clean Earth Magnet® technology, Niron Magnetics (Minneapolis, Minn.; www.nironmagnetics.com) has demonstrated its novel magnet-production technology at the pilot scale, and plans to open a full-scale manufacturing facility in Sartell, Minn., which will significantly scale up production.

"The process begins with the creation of precisely engineered iron oxide nanoparticles, which undergo a specialized reduction process that results in iron nitride nanoparticles. The final step involves aligning the magnetic particles and compacting them under high pressure to form dense permanent magnets," explains Frank Johnson, CTO of Niron Magnetics.

Currently, the company operates out of their commercial pilot plant in Minneapolis, which has a capacity of 5 tons/yr of REE-free magnets, but the new plant is expected to produce 1,500 tons/yr by 2026. "Companies like General Motors, Volvo, Samsung and Stellantis have invested in Niron's technology. These partnerships are extremely important for developing applications that leverage iron nitride's unique magnetic properties, enabling manufacturers to reduce their reliance on rare-earth materials while maintaining high performance standards," adds Jonathan Rowntree, CEO of Niron Magnetics.

Additionally, says Rowntree, Niron's magnets are made with iron nitride, which "boasts the highest theoretical magnetization of any known material," while also providing superior thermal stability when compared to traditional rare-earth-based magnets.

### DESALINATION ADVANCES

Water scarcity is a growing global concern that is driving increasing efforts to conserve, re-use and treat water. Desalination of seawater is a known technology to combat water shortages, but it is an energy-intensive process. Solar-powered evaporation can be a more energy-efficient desalination process, as demonstrated by researchers from the University of South Australia (UniSA; www.unisa.edu.au). The salt in seawater, however, limits the achievable evaporation rate. Studies reportedly found seawater evaporation rates to be about 8% lower than those for pure water.

Professor Haolan Xu, a materials science researcher at UniSA, in collaboration with researchers from China, has developed a simple strategy to overcome this limitation. The team was able to achieve seawater evaporation rates 18.8% higher than for pure water by introducing common clay minerals into a floating photothermal hydrogen evaporator. According to the researchers, the hydrogen evaporator maintained its performance for months after immersion in seawater. The mineral materials used in the process included halloysite nanotubes (HNTs), bentonite (BN), zeolite (ZL) and montmorillonite (MN) in combination with carbon nanotubes (CNTs) and sodium alginate (SA) to form a photothermal hydrogel.

"The key to this breakthrough lies in the ion exchange process at the air-water interface," Xu says. "The minerals selectively enrich magnesium and calcium ions from seawater to the evaporation surfaces, which boosts the evaporation rate of seawater. This ion-exchange process occurs spontaneously during solar evaporation, making it highly convenient and cost-effective."

This work has been published in the journal *Advanced Materials*.

### HIGH-PRESSURE $H_2$ PRODUCTION

Clyde Hydrogen Systems (Glasgow, Scotland; www.clydehydrogen.com), a spinout company from the University of Glasgow's School of Chemistry, has announced the successful production of hydrogen at pressures exceeding 100 bars using its scaled-up catalytic hydrogen generator. The company's technology uses a decoupled electrolysis process that includes an electrochemical reductor that generates a reduced mediator solution and a catalytic hydrogen generator that produces high-pressure hydrogen gas. The business is on track to deliver a fully integrated pilot system by late 2025. ❐

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## Plant Watch

### Chevron upgrades Pasadena refinery to increase capacity and flexibility

December 11, 2024 — Chevron Corp. (Houston; www.chevron.com) has completed a retrofit of its petroleum refinery in Pasadena, Texas, which is expected to increase product flexibility and expand the processing capacity of lighter crude streams by nearly 15% to 125,000 barrels per day (bbl/d). The phased startup of the upgraded asset is expected to last through the first quarter of 2025.

### PCC Group to build chlor-alkali facility at Chemours plant in Mississippi

December 11, 2024 — The Chemours Co. (Wilmington, Del.; www.chemours.com) announced that PCC Group SE (Duisburg, Germany; www.pcc.eu) plans to build and operate a chlor-alkali facility on the grounds of Chemours' titanium dioxide plant in DeLisle, Mississippi. The new facility will have an annual nameplate capacity of up to 340,000 metric tons per year (m.t./yr) once the plant is operational. Construction is expected to begin in early 2026 with startup in 2028.

### BASF starts up its expanded ammonium chloride plant in Ludwigshafen

December 11, 2024 — BASF SE (Ludwigshafen, Germany; www.basf.com) has expanded the production capacity of ammonium chloride at its Ludwigshafen site, increasing capacity by 50% and improving product quality. Industrial applications for ammonium chloride include the production of batteries, galvanized metals and cleaning agents and process chemicals for the chemical, cosmetic and pharmaceutical industries.

### Yara begins production of renewable ammonia in Brazil

December 10, 2024 — Yara International ASA (Oslo, Norway; www.yara.com) said that it has become the first company in Brazil to produce ammonia from renewable biomethane made from sugarcane waste. Yara's industrial complex in Cubatão, the largest consumer of natural gas in São Paulo and Brazil's leading ammonia producer, is now fully equipped to operate with biomethane feedstock.

### Production of $CO_2$-based carbonates starts up in China

December 5, 2024 — Asahi Kasei Corp. (Tokyo; www.asahikasei.com) announced that Jiangsu Sailboat Petrochemical started commercial operation of a new carbonates plant in Lianyungang, Jiangsu Province, China. The plant uses technology licensed from Asahi Kasei for the production of high-purity ethylene carbonate (EC) and dimethyl carbonate (DMC) with $CO_2$ as a main raw material. The plant has the capacity to use 54,000 m.t./yr of $CO_2$ as feedstock. EC and DMC are essential materials for the production of lithium-ion battery electrolytes.

### Fujifilm to expand production capacity for CMP slurries

December 5, 2024 — Fujifilm Corp. (Tokyo; www.fujifilm.com) will increase its production capacity of chemical mechanical planarization (CMP) slurries, which are advanced semiconductor materials, at its production site located in Kumamoto Prefecture, Japan. Fujifilm also operates CMP slurry production sites in the U.S., Taiwan and South Korea.

### UBE to increase production capacity for high-purity nitric acid

December 2, 2024 — UBE Corp. (Tokyo; www.ube.com) announced plans to increase the production capacity of high-purity nitric acid at the UBE chemicals site in Yamaguchi Prefecture, Japan. The market for high-purity nitric acid, which is used for semiconductor cleaning and in the etching process, has been experiencing continuous growth in recent years. This expansion is expected to increase capacity by around 30% compared to current levels.

### Air Liquide will build hydrogen production unit at TotalEnergies biorefinery site

November 27, 2024 — Air Liquide (Paris, France; www.airliquide.com) recently announced a renewable-hydrogen production project at TotalEnergies' (Courbevoie, France; www.totalenergies.com) La Mède site in the Provence-Alpes-Côte d'Azur region in France. The new site will have a capacity of 25,000 m.t./yr of renewable hydrogen produced from recycled biogenic byproducts from the TotalEnergies biorefinery, instead of using fossil-based hydrocarbons as feedstock. The renewable hydrogen will be used mainly by the biorefinery for the production of biofuels.

## Mergers & Acquisitions

### Dow to sell 40% stake in U.S. Gulf Coast infrastructure assets

December 11, 2024 — Dow (Midland, Mich.; www.dow.com) announced that it has entered into a definitive agreement to sell a 40% equity stake in select U.S. Gulf Coast infrastructure assets to a fund managed by Macquarie Asset Management, a global infrastructure and energy asset manager. Dow expects to receive initial cash proceeds of approximately $2.4 billion from the transaction. This new partnership between Dow and Macquarie will create a specialist infrastructure provider to Dow and other industrial customers at its five locations in Texas and Louisiana.

### Hexion acquires autonomous manufacturing firm Smartech

December 6, 2024 — Hexion Inc. (Columbus, Ohio; www.hexion.com) has acquired Smartech, a technology company specialized in autonomous manufacturing solutions that combine artificial intelligence, advanced control systems and process optimization algorithms. Smartech's systems target the production of waxes, phenol-formaldehyde (PF) resins, methylene diphenyl diisocyanate (MDI) resin and more, and are expected to strengthen Hexion's position in the adhesives, construction and building materials sectors.

### Dow sells flexible packaging adhesives business to Arkema

December 5, 2024 — Dow has completed its previously announced sale of the company's flexible-packaging laminating adhesives business, within Dow's Packaging & Specialty Plastics segment, for $150 million, to Arkema S.A. (Colombes, France; www.arkema.com). The sale includes five manufacturing sites in Italy, the U.S. and Mexico. The business includes solvent-based and solventless laminating adhesives and heat-seal coating product portfolios.

### Ineos sells composites business for €1.7 billion

December 5, 2024 — Ineos Enterprises Ltd. (London; www.ineos.com) entered into an agreement for the sale of the Ineos Composites business to KPS Capital Partners, L.P. for an estimated consideration of around €1.7 billion at completion. The business has combined sales of more than €800 million per year and operates 17 facilities and 3 technology centers in Europe, North and South America, Asia and the Middle East. Ineos Composites is a global manufacturer of unsaturated polyester resins, vinyl ester resins and gelcoats used in the production of plastic composites for a wide range of applications.

### Corteva and bp plan JV for biofuel feedstocks

December 2, 2024 — Corteva Inc. (Indianapolis, Ind.; www.corteva.com) announced a collaboration with bp plc (London; www.bp.com) related to the companies' intent to form a joint venture (JV) focused on crop-based biofuel feedstocks. The JV aims to progressively scale up volumes, reaching delivery of 1 million m.t./yr of biofuel feedstocks for SAF production by the mid-2030s. The two companies anticipate finalizing definitive agreements in 2025 with the target operational date for the JV later in the year.

### Honeywell to sell PPE business for $1.3 billion

November 22, 2024 — Honeywell International, Inc. (Charlotte, N.C.; www.honeywell.com) agreed to sell its Personal Protective Equipment (PPE) business to Protective Industrial Products, Inc., a portfolio company of Odyssey Investment Partners, for $1.325 billion in an all-cash transaction. The PPE business, part of Honeywell's Industrial Automation (IA) business portfolio, currently operates 20 manufacturing sites and 17 distribution sites across the U.S., Mexico, Europe, North Africa, Asia Pacific and China. ■

*Mary Page Bailey*

# Weighing in on Accuracy

## Innovation, intelligence and automation increase precision in weighing equipment for chemical processors

Accurate weighing and dosing are critical to the success of any chemical process, because they ensure product quality, safety and resource optimization. Fortunately, innovative technologies, intelligence and automation are helping processors boost accuracy and precision in their weighing operations. Here, industry experts "weigh" in on the benefits of these developments.

"Whether used in food, pharmaceuticals, chemicals or other industries, accurate ingredient weighing is a critical component in assuring product quality, consistency and safety," says Joe Schobel, sales engineer for chemicals with AZO (Memphis, Tenn.; azo-inc.com). "Each ingredient's proportion within a mixture contributes to the product's finished quality, so any deviation can offset the delicate balance of a precise formulation."

Keith Melton, sales manager for the battery industry with Coperion K-Tron (Niederlenz, Switzerland; coperion.com), agrees: "High feeding accuracy is of paramount importance in a range of chemical manufacturing applications, including production of battery active materials and pharmaceutical manufacturing.

"First, it ensures the consistency and quality of the final product by maintaining precise proportions of the various chemical components. This is crucial, as even slight deviations can lead to significant changes in product properties," Melton continues. "Second, it enhances efficiency by minimizing waste of raw materials, thus reducing production costs. Additionally, high feeding accuracy is vital for safety reasons, as incorrect proportions can lead to hazardous reactions or the production of harmful byproducts. Therefore, accurate weighing and feeding systems are indispensable in chemical production applications for ensuring product quality, cost effectiveness and safety."

### Addressing weighing challenges

There are a variety of challenges and needs when trying to provide high-accuracy weighing performance in the chemical process industries (CPI). Vibrations are one of the greatest challenges, while precision in minor and micro dosing, development of new technologies for emerging battery applications and more modernized laboratory weighing equipment are also on the list of demands, according to the experts. As a result, weighing technology providers are working on equipment innovations and enhanced intelligence and automation designed to help minimize challenges and fulfill the requirements of weighing technologies for chemical processes.

***Managing vibration.*** "Environmental factors, such as vibrations from nearby operating equipment, can impact the ability of the weighing system to provide an accurate weight signal," says Coperion's Melton. "Recognizing that the weighing system must be able to understand the difference between environmental influences and the actual weight to be measured has led to the development of a number of solutions that address these issues."

To help the feeder control discriminate between actual weight data and the contaminating effects of inertial forces resulting from ambient vibration, the Coperion Smart Force Transducer (SFT) weighing technology (Figure 1) and KCM feeder control modules were developed. "The SFT weighing technology ensures precise and accurate measurements, which are crucial for maintaining optimal productivity and reducing waste," says Melton. "At the same time, our KCM feeder control modules play a pivotal role in controlling and managing the feedrate. Together, these two components ensure our systems operate efficiently and effectively, delivering high-quality results consistently, even in difficult plant environments."

Also addressing vibration in weight-based control of highly integrated and stand-alone applications is Hardy Process Solution's 6850 weight controller (Figure 2). "It's the first weighing instrument of its kind featuring dual core processing," says Tim Norman, senior product development manager with Hardy Process Solutions (San Diego, Calif.; hardysolutions.com). "It was designed this way so one core can be used to run an application, such

Source: Coperion K-Tron

**FIGURE 1.** Coperion K-Tron's Smart Force Transducer (SFT) technology delivers high-precision weighing, even in difficult plant environments

as dispensing or filling, and the other core is dedicated to digital signal processing, to eliminate the effects of mechanical vibrations on a scale system. This is important because vibrations contribute to inaccuracies, therefore eliminating vibration improves not only the process, but product quality, as well."

***Higher accuracy in smaller doses.*** Because inaccuracy in micro and macro weighments can have a significant influence on reactions or alter a product, there has been a demand for more accuracy in these measurements, says AZO's Schobel. Fortunately, innovation and automation can provide solutions for these applications. AZO's Componenter (Figure 3) batching equipment offers a highly accurate, automated dosing and weighing system for minor and macro ingredients. Raw materials are fed into the top of the Componenter system and stored. The middle of the system is where the metering, dosing and weighing of ingredients takes place and the bottom of the system is where ingredients are fed into the next processing step.

"Whether you produce food, pharmaceuticals, chemicals or plastics, this batching equipment can automate the process, which helps eliminate errors and inaccuracies associated with manual operations, reduces the risk of contamination in the process and simultaneously weighs and discharges ingredients with high accuracy for faster throughput," says Schobel.

Also recognizing a similar need for precision weighing of small components, especially in the rubber and tire industries, Zeppelin Systems (Friedrichshafen, Germany; zeppelin-systems.com) offers the Automated Small Components Weighing System (ASCW) for fully automated weighing of granular or powdery bulk materials with different densities and flow characteristics and for providing mixtures of bulk materials, which are required in rubber blends.

"The ASCW is available with up to 40 different material hoppers mounted in a row, and is suitable for big-bag and bag feeding," explains Nicole Werner, product and technology manager with Zeppelin Systems. "Equipped with a double dosing screw with a shut-off valve or vibrating chute with a catch gate and GiW [gain-in-weight] scales integrated in a surrounding roll conveyor, the roll conveyors move multiple batch-collecting buckets prepared with bag inlays along the row of material hoppers. The buckets stop below the material hoppers, are lifted and then balanced by the corresponding scale below. All materials get dosed and weighed into the buckets at the same time until the set values are reached. The clocked dosing will repeat until the first bucket reaches the ejection position, where a bag inlay is removed and the bucket moves onto the bag insertion to start a new dosing cycle.

"Optional features, such as automated bag insertion, bag sealing, labeling and bag handling, are available to fully automate the dosing and weighing process of up to 25-kg batches with a capacity of up to 2,400 batches per day," she says.

***Developments for emerging applications.*** Battery production is a fast-growing sector, however, the production of battery cathode material is a lengthy and complex process and any fluctuations along the process chain can result in problems, such as subpar end-product quality, plant downtime and wasted material, says Coperion's Melton. "One parameter that can be controlled is the addition of ingredients. To ensure a steady flow of material, high feeding accuracy is essential or, at the least, high measurability of the added ingredients is desirable.

"The focus is usually less on weighing accuracy and more on the accuracy of the delivered sample, often expressed in terms of two-sigma accuracy," Melton explains. "For continuous processing, this becomes even more complex, with two-sigma based on a typical sample time of 30 to 60 seconds and increasingly moving towards shorter 5- to 10-second sample times. Naturally, achieving higher accuracies becomes more challenging with shorter sample times, making consistent short-term accuracy of the weighing system crucial."

On the feeder side, the battery industry has a specific need for dry coating applications. "Accuracy is


Source: AZO

**FIGURE 3.** AZO's Componenter batching equipment offers a highly accurate, automated dosing and weighing system for minor and macro ingredients

Source: Hardy Process Solutions

**FIGURE 2.** Hardy's 6850 series weight controllers are suitable for a variety of weight-based applications. The weight controller features a dual-core processor and combines direct process control with fast, accurate and stable weight data, which is essential to profitable manufacturing operations

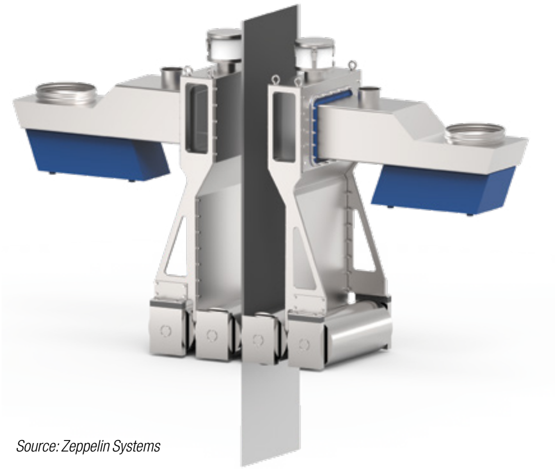


**FIGURE 4.** With the Feeding & Dosing Unit, Zeppelin Systems has developed an automated system that ensures a constant and evenly distributed material flow to the calender to enhance battery production

a crucial factor in this continuous process, because a consistent, thin layer must be applied to achieve the desired result. Dry coating requires a continuous distribution at the outlet, such that the entire width of a calender roll holds the same amount of material. The accuracy is measured across 20- to 50-mm increments, based on the two-sigma/time model, and presents a significant challenge not only for the weighing system but also for the mechanical device," says Melton. "Coperion has developed a completely new type of feeder to answer this need. Called the Coperion K-Tron Roller Feeder, it will be launched in the new year."

Similarly, Zeppelin Systems is developing sustainable and digitalized machinery for battery production with a focus on a feeding and dosing unit that ensures a constant and evenly distributed feed of premixed and conditioned dry battery mass to the calender, says Werner.

For dry battery production of battery electrodes, the pre-treated anode or cathode bulk material mixtures must be transferred into the inlet of a calender, she explains. In general, a calender consists of several rotating cylindrical rollers that press the bulk material into a thin film, which is then laminated onto a metal foil to subsequently create the battery electrode. Normally, the flow behavior of the solid mixtures is rather poor. The finished electrode material is difficult to handle due to the binder content and smaller particle diameter. The electrode materials are very sensitive, so even minimal external forces, pressure and increased temperatures may cause the materials to compact into pasty lumps. Because of this, no standard solutions for storage and feeding to the calender can be used.

"However, with the newly developed Feeding & Dosing Unit (FDU) (Figure 4), Zeppelin Systems has solved a challenging task by developing a system that ensures a constant and evenly distributed material flow to the calender," says Werner. "Thanks to a special design and constant level control, the unit provides a fully automated solution to connect to upstream processes and to allow material storage without risk for bridging."

## Modern laboratory weighing

Modern weighing technologies are also evolving to address the growing complexity and demands of CPI laboratories, according to Lucas Foerster, product manager, laboratory weighing applications, with Sartorius AG (Göttingen, Germany; sartorius.com). "Several advancements stand out for their ability to overcome challenges and satisfy user needs."

Among them are sensor and software innovations. "New lab balances are equipped with advanced sensors and software to monitor ambient conditions, such as temperature, humidity and air pressure, that can affect weighing accuracy," says Foerster. "These systems either compensate for adverse effects or alert users when conditions might compromise results, ensuring reliable performance, even in suboptimal lab environments."

Modern weighing technologies, such as those found in the Sartorius Premium Lab Balance Cubis II Portfolio (Figure 5), enhance both product quality and laboratory productivity by providing faster and more stable measurements and reducing inaccuracies, even in challenging conditions. And, the seamless software integration and guided protocols allow laboratories to streamline workflows, maintain efficiency and focus on critical analysis.

"Further, product quality can be significantly enhanced by using balances that comply with 21 CFR Part 11 requirements. These balances feature robust capabilities, such as user management, electronic signatures, alibi memory for secure storage of every weighing value and comprehensive audit trails," says Foerster. "These functions ensure data integrity by safeguarding all generated data against manipulation, ultimately supporting high product quality and regulatory compliance."

## Innovation and automation

While every weighing operation differs based on the product being produced and the process environment, modern weighing, feeding and dosing systems that include innovative technologies and automation to enhance accuracy provide significant benefits to weighing applications.

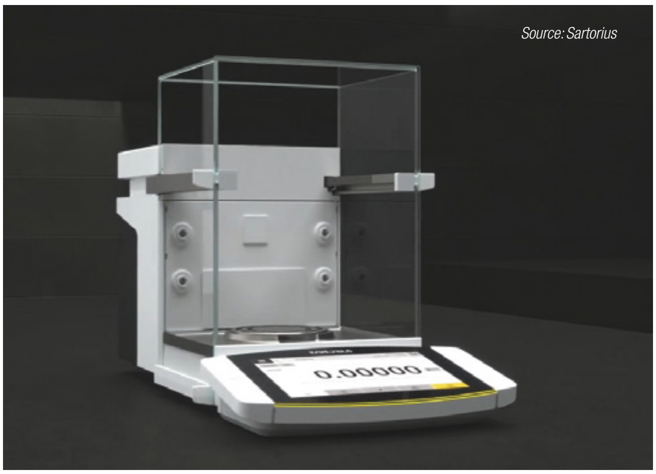


**FIGURE 5.** The Sartorius Premium Lab Balance Cubis II Portfolio enhances both product quality and lab productivity by providing faster and more stable measurements and reducing inaccuracies, even in challenging laboratory conditions

Precise weighing delivers accurate ingredient proportions, which ensures consistency and quality. Automation removes the element of human error from the process and eliminates quality variations due to inconsistent ingredient ratios. "In addition," says Hardy's Norman, "Today's equipment can include advanced diagnostics. When the ability to predict that a scale might need to be calibrated or checked for issues is combined with advances in edge computing and smarter algorithms, users can monitor scale conditions for trouble before issues become critical and adversely affect the process."

Modernization and automation also boost efficiency and speed up the production process in several ways. Automation allows processes to run 24/7, if needed, and production never has to stop due to lack of ingredients. In addition, modern equipment offers faster response times to changes in weight, says Hardy's Norman. "The scales of yesterday would update a weight measurement every second or so, but today we are able to read signals from sensors at 4,800 signals per second. This means the weight data sent to control systems can be used to make real-time decisions, such as opening or closing a valve in a process, at precisely the right time. This leads to increased efficiency, as well as better product consistency, less waste and ultimately higher product quality."

System optimization is also possible with advanced intelligence options. "Controllers are now able to 'learn' from the data that is collected during operation of the system and apply this to improve the process," explains Coperion's Melton. "One challenging aspect of this involves determining how to use accurate weighing data effectively. This requires not only real-time monitoring but also the integration of past experience values, making a controller truly intelligent. While we haven't yet incorporated AI [artificial intelligence] into feeding, we offer a variety of smart features."

Melton says controllers are programmed to manage not only general control and process performance, but also to manage unexpected events, thereby preventing disturbances from causing weighing errors and subsequent poor quality in the final product.

Higher levels of accuracy presented by automation are also minimizing waste in the industry. "More accurate weighing involves not just controlling, but also precisely measuring process parameters. It's also important to eliminate environmental influences that could affect the accuracy of these measurements," says Melton. "By doing so, waste can be significantly reduced, leading to more efficient operations, lower costs and higher productivity."

Production flexibility is also enhanced with modern automated systems. As they are adaptable to diverse production needs, automated weighing systems can accommodate changes in batch sizes and material variations. Flexibility is critical in new product formulations or in environments where fluctuations in material characteristics due to humidity or clumping during storage occur, say the experts at AZO. ■

*Joy LePree*

# Flowmeters

*Emerson*


*Binmaster*

*Fluid Components International*

## This flowmeter is designed for demanding applications

Measuring volumetric flow accurately and reliably is difficult for applications where the process liquid is highly viscous, extremely abrasive, prone to plugging, at high temperature, or a combination of these conditions. In applications with low ambient temperatures, hot process media, or a combination of both, heat tracing is often required, necessitating supply of electrical power, and creating a maintenance-intensive single point of failure. The Rosemount 9195 Wedge Flowmeter (photo) addresses these and other common measurement challenges with its unique design. The wedge element itself has no small passages that could plug due to entrained particles, and it is abrasion-resistant due to the shallow approach angle of the process liquid and the lack of critical sharp edges. Highly viscous liquids are measured accurately due to the linear response of the meter, even at low Reynolds numbers. The sensor's operating temperature range is –40° to 1,000° F(–40° to 538°C), and the meter is available with a thermal range expander for measuring hot or viscous liquids without the need for heat tracing. Available line sizes for the sensor are 2 to 8 in. (50 to 200 mm). All wetted materials are 316L stainless steel, and the meter complies with ASME B31.3 and CRN safety standards. — *Emerson, Shakopee, Minn.*
**www.emerson.com**

## A device for detecting no-flow conditions in solids-handling

The Flow Detect 2000 (photo) is a non-intrusive instrument for detection of no-flow conditions in solids-handling equipment, such as distributors, conveyors, pipelines, gravity chutes, feeders and bucket elevators. The reliable device works by emitting a low-power microwave signal at a material and detects the reflected waves. By monitoring the frequency difference between the emitted and reflected signals, the Flow Detect 2000 can sense flow/no-flow conditions. The instrument prevents downtime caused by material blockages, conveyors running empty, lack of material flowing to and from a process, and loose slide gates. The Flow Detect 2000 helps prevent cross-contamination of materials, avoids product waste and prevents improper batching. It has a single-piece design that eliminates the need for a separate controller and makes no direct contact with the material flow stream. — *Binmaster, Lincoln, Neb.*
**www.binmaster.com**

## A remote-mountable flowmeter is for hard-to-reach locations

The ST75 Series Flowmeter (photo) offers a remote-mountable, space-saving configuration that solves piping layout issues in potentially hazardous areas or hard-to-reach locations crowded with equipment. The device offers direct mass-flow measurement, and is ideal for a wide range of industrial applications, including burner and boiler fuel and air feed lines, industrial furnaces, kilns and oven fuel/air controls, natural gas sub-metering, chiller air-flow measurements, dosing and gas injection rate controls, air compressor system control and point-of-use monitoring, and co-gen and turbine generator fuel-flow measurements. These in-line (spool-piece) style flowmeters have no moving parts and are available for use in pipe diameters from 0.25 to 2 inches. The ST75 flowmeter's transmitter/electronics can be integrally mounted with the flow element (probe), or it can be remote mounted to best match the installation situation. The remote mount transmitter, which includes a full digital display, can be mounted up to 50 feet (15 meters) away from its thermal mass-flow sensor in the process piping and connected via two 0.50-in. FNPT or M conduit connections. — *Fluid Components International, San Marcos, Calif*.
**www.fluidcomponents.com**

## This display transmitter shows flowrate and totalized flow

The SumoFlo CELE-8103-D integral display transmitter (photo) simultaneously shows flowrate, totalized flow, temperature and product density in life science biopharmaceutical applications. The transmitter is designed to be integrated into this company's SumoFlo single-use Coriolis flowmeters. The SumoFlo CELE-8103-D Display Transmitter features a 144×144-mm four-line display and is available in both panel-mounted and tabletop configurations. The SumoFlo CELE-8013's display never comes into contact with fluids, making it a durable component that can be reused in future applications. The display transmitter is also designed for ease of use, with the unique capability to re-zero or reset the totalizer directly from the front panel. In total, the SumoFlo CELE-8103 Integral Display Transmitter provides users with instantaneous process metrics, enabling biopharmaceutical processors to identify and respond to process variations quicker, with fewer wasted materials and less downtime, according to the company. — *PSG Biotech, Oakbrook Terrace, Ill.*
**psgdover.com/biotech**

## A flowmeter for precise measurement of hydraulic fluid

The HM-U Hydraulic System Flow Meter (photo) is a cost-effective and versatile turbine-style flowmeter that measures hydraulic fluids for precise regulation and control of flowrates in hydraulic systems. It is optimized for hydraulic performance applications and ideal for components such as pumps, valves and fittings. The HM-U Hydraulic System Flow Meter performs in temperature ranges from –40°F (–40°C) to 248°F (120°C) and offers accuracy of ±0.5% M.V. over its full range with 30-cP fluid. Two integrated 0.25-in. BSPP (British standard parallel pipe) connections allow users to install their own temperature and/or pressure transmitters for optional measurement. Compact and lightweight, the flowmeter features a durable aluminum housing with stainless steel internals. The HM-U Hydraulic System Flow Meter is compatible with this company's EDGE Flow Sensor that offers Bluetooth capabilities, providing users easy access, understanding and control of their flow measurement. Easily mounted on the turbine flowmeter, the EDGE Flow Sensor outputs a frequency, current, or analog signal that gives users more installation flexibility, especially when unsure of readout equipment or a control room interface. — *AW-Lake, Oak Creek, Wis.*
**www.aw-lake.com**

## This electromagnetic flowmeter expands measurement options

To achieve the goal of developing a modular electronic control solution with maximum flexibility that is equally suitable for all applications and media without compromising on precision or material resistance, this company has introduced the MIK electromagnetic flowmeter (photo) using the new U-PACE compact electronics. This set of electronics takes over the flow display and dosing simultaneously, instead of having to use separate evaluating electronic devices. To ensure the flexibility of the new development, a chemically resistant flowmeter and precise flow monitor have been combined in one device and optimized for a wide range of applications. This makes the MIK suitable for almost all applications such as flow measurement, flow control, filling and quantity recording, for example in the food, chemical and paper industries, as well as for aggressive fluids found in the construction industry. The measuring ranges are generously designed from 0.01 to 700 L/min and are suitable for all requirements. The MIK is insensitive to changes in viscosity, density, temperature or pressure and generates negligible pressure loss. At the same time, the instruments are resistant to corrosive acids and alkalis thanks to optional material combinations. The U-PACE electronics use the proven IO-Link technology, a standardized and real-time capable communication standard for connecting sensors and actuators to an intelligent automation system. This makes it possible to connect the measurement technology to almost all common processes and system concepts and, with its short response times, represents real added value. — *KO-BOLD Messring GmbH, Hofheim am Taunus, Germany*
**www.kobold.com** ■

*Scott Jenkins*

*PSG Biotech*


*AW-Lake*


*KO-BOLD Messring GmbH*

# Accelerating Materials Development with AI

*Department Editor: Scott Jenkins*

Advanced materials are considered to be core enablers for technologies aimed at broad global concerns, such as climate change, sustainable manufacturing, critical-materials supply chains, environmental mitigation and remediation and others [*1*]. The process by which novel advanced materials are designed and developed is accelerating through the use of a raft of technologies, including those in artificial intelligence (AI) and robotics, and has been enabled by the expansion of high-performance computing and cloud-based data infrastructure. This one-page reference provides an overview of how machine learning and other AI approaches are accelerating materials development.

Advanced materials are aimed at improving the performance of a product or process. Properties targeted include weight, strength, durability, conductivity, stability, self-healing capability and more [*2*]. Advanced materials may include alloys, coatings, catalysts, composite materials and two-dimensional materials like graphene, as well as nanoscale materials, like quantum dots.

## AI-enabled materials development

Purely experimental approaches to discovering new materials has been relatively slow, so researchers have turned to computational approaches to keep up with demand for new materials. Although it is a tool rather than a panacea, AI provides a number of exciting opportunities for materials research. In general, a machine-learning model of a material can be developed to provide predictive capabilities where traditional, physics-based models either do not yet exist, or remain so challenging (and slow) as to be too expensive in time or other resources [*1*]. AI models can aid in the development of new physical models by elucidating previously hidden, complex relationships. Similarly, sophisticated use of AI tools will open opportunities for understanding increasingly complex systems.

AI has been employed in advanced-materials in a number of ways, including the following [*3*]:

- Materials property and performance prediction, given a set of input parameters (including processing history and service conditions, for example)
- Discovery of new material compositions and processing routes for achieving application-oriented targets in terms of desired material properties
- Image-based analysis methods for automating materials characterization

To support the use of machine learning in the design and development of advanced materials, a number of broad initiatives have been launched. Several examples are described in Table 1. ■

**TABLE 1. LARGE-SCALE MATERIALS INITIATIVES**

| | |
|---|---|
| **NIST JARVIS**<br>jarvis.nist.gov | The JARVIS (Joint Automated Repository for Various Integrated Simulations) is a repository designed to automate materials discovery and optimization using classical force-field, density functional theory, machine learning calculations and experiments. It is administered by the National Institute of Standards and Technology (NIST) [*4*]. |
| **Materials Genome Initiative**<br>www.mgi.gov | The Materials Genome Initiative (MGI) is a U.S. federal multi-agency program launched in 2011 to accelerate the discovery, design, development, and deployment of new materials at a fraction of the cost, by harnessing the power of data and computational tools in concert with experiments [*1*]. Modeled after the Human Genome Project (1990–2003) and including military, scientific and executive branch partners, the MGI has three broad goals: Unify the materials innovation infrastructure; Harness the power of materials data; and Educate, train and connect the materials R&D workforce. |
| **Citrine Informatics Generative AI platform**<br>citrine.io | Citrine Informatics is the creator of the Citrine Platform, an AI platform for data-driven materials and chemicals development. Citrine Informatics began in 2013 as a system designed to combine smart materials data infrastructure and AI. The objective is to accelerate development of cutting-edge materials, facilitate product portfolio optimization and codify a company's research intellectual property, enabling its reuse and preventing its loss [*5*]. The platform is designed for wide use, and is supported by a team of experts to help users take AI to scale. |
| **The Institute for AI-Enabled Materials, Discovery, Design, and Synthesis (AIMS)**<br>icds.psu.edu | AIMS is a collaboration of researchers from Penn State University, MIT and the University of Wisconsin-Madison. AIMS will "catalyze and establish interdisciplinary and transdisciplinary collaborations that transcend institutional and organizational boundaries." The initiative is also concerned with preparing an AI-savvy materials-discovery workforce by training a diverse cadre of individuals. In addition to AI advances and technologies that enable new materials design, discovery and synthesis, AIMS will also provide organizing frameworks, infrastructure, collaborative human-AI systems and tools. |
| **AI4Science Initiative**<br>ai4science.caltech.edu | AI4Science is an initiative at the California Institute of Technology (Pasadena, Calif.; www.caltech.edu) led by Anima Anandkumar and Yisong Yue that aims to bring together AI researchers with experts from other disciplines to push modern AI tools into every area of science and engineering. Launched in the summer of 2018, the initiative organizes talks, courses and tutorials aimed at training researchers from across the scientific spectrum in the theory and practice of machine learning algorithms. |
| **The Materials Project**<br>Next-generation.materialsproject.org | The Materials Project is a multi-institution, multi-national effort to compute the properties of all inorganic materials and provide the data and associated analysis algorithms for every materials researcher free of charge. The ultimate goal of the initiative is to drastically reduce the time needed to invent new materials by focusing costly and time-consuming experiments on compounds that show the most promise computationally. |
| **Google GNoME algorithm**<br>deepmind.google | Google DeepMind's Graph Networks for Materials Exploration (GNoME) uses state-of-the art graph neural networks (GNNs) that improve modeling of material properties given structure or composition. |
| **Johns Hopkins Applied Physics Laboratory**<br>jhuapl.edu | The JHU-APL program Accelerating Materials Discovery for National Security seeks to leverage AI in reimagining and accelerating the targeted discovery of materials that are "tailored to withstand and perform under the most demanding conditions." |

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# Troubleshooting a Trayed Distillation Column

Presented here is the progress and resolution of a troubleshooting case involving a distillation column with a capacity reduction problem

**Sebastian Löw and André Ohligschläger**
Nobian GmbH
**Vijaya Bhaskar Reddy Gummala, Tim Rogalinski and Ralf Ziegler**
Siemens AG

Troubleshooting distillation columns during operation is often the key to stable production at industrial facilities. The collection of troubleshooting references from Kister [*1*] and others [*2, 3*] show the value of reference cases for the industry, not only during the troubleshooting process, but also when it comes to decision making on how to identify the problem. This article presents a unique troubleshooting case of a trayed distillation column with a diameter of 1.8 m comprising 86 trays. During the startup of the distillation column after a periodic turnaround in December 2019, the reboiler leaked and the column capacity dropped significantly, even after the redundant reboiler was taken into operation. A qualitative data analysis was performed, comparing the current capacity of the column to that of the capacity before the turnaround. The analysis showed that above a certain feed rate, this distillation column's products did not meet specifications, resulting in less product than in the years before the reboiler leakage.

An inner inspection of the column during normal operation was not feasible to investigate the cause of the capacity reduction, because it would require a total plant shutdown for more than a week. This article discusses how gamma scanning and hydraulic rating of the trayed column enabled engineers to identify the cause of the capacity reduction, and how reboiler leakage could lead to a significant reduction in column capacity.

## Column configuration

This distillation troubleshooting case refers to a chloromethane purification column that has been in operation since the early 1990s. The desired product is separated at the top of the column from the higher-boiling chlorinated hydrocarbons, and the bottoms are fed to a downstream column. Figure 1 shows the column configuration. The material of construction of the column is carbon steel, and according to wall-thickness measurements,

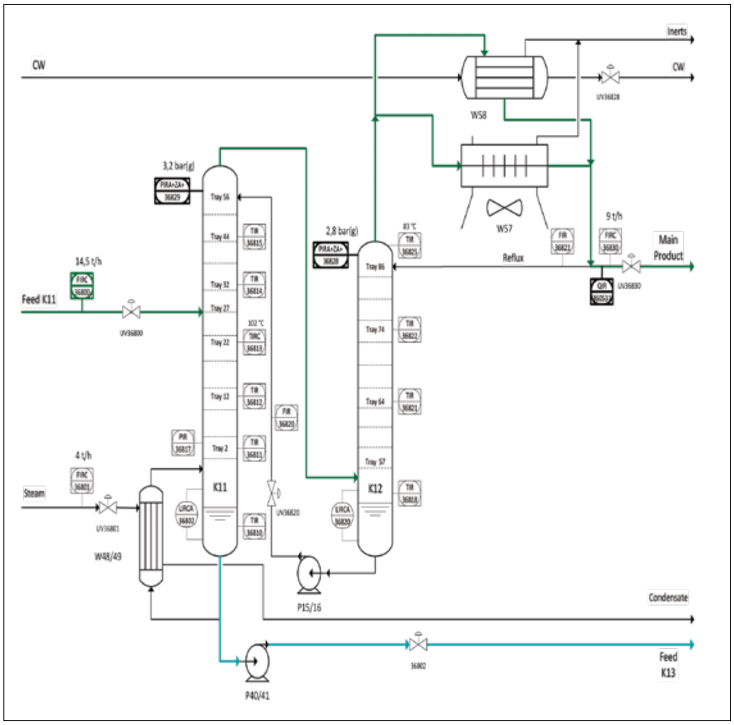


**FIGURE 1.** The configuration of the chloromethane purification column is shown here

IN BRIEF

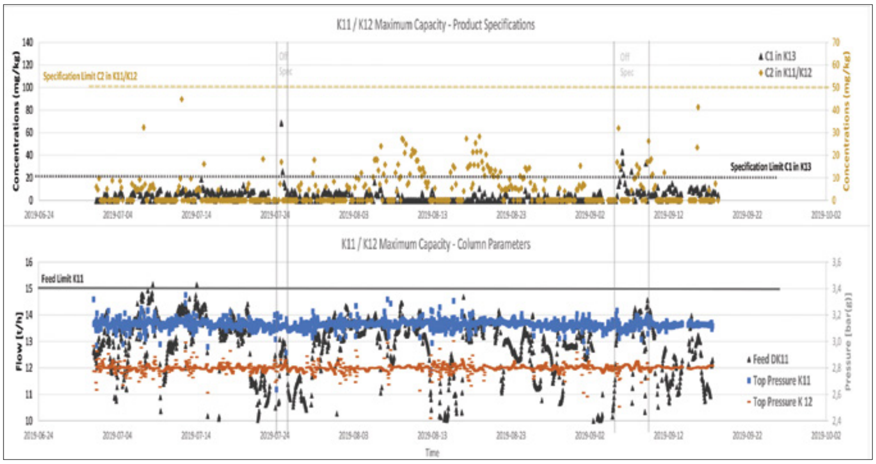

**FIGURE 2.** The column profiles, including feed flow, overhead pressure and concentration, are shown here before the turnaround

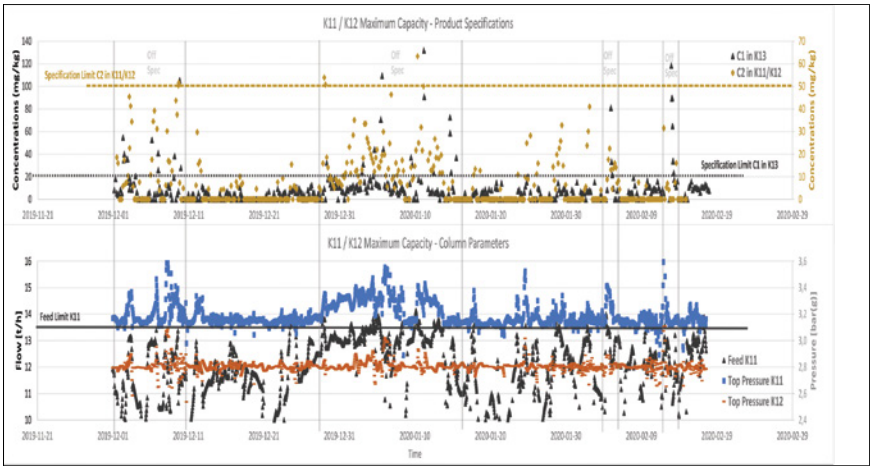

**FIGURE 3.** Changes in the column profiles after the turnaround are displayed here

the corrosion rates are very low.

The column has a diameter of 1.8 m and in total, 86 single-pass trays are installed. To reduce the height and to fit inside a production building, the column is divided into two towers. In the first tower, (K11; tray numbers 1 to 56), standard float valves (Ballast® V1 and V1X) are installed, and the second tower (K12; tray numbers 57 to 86) is equipped with caged valves (Varioflex® type VV16–3L20). The stripping section in K11 from tray 1 to 28 has a tray spacing of 300 mm, and the rectification section (trays 28 to 86) is distributed among the two towers with tray spacings of 250 mm in the K11 tower and 300 mm in K12.

Vertical thermosiphon reboilers operated with condensing steam attached to the first tower serve as the energy source for the separation. An air-cooled heat exchanger and a water-cooled heat exchanger are installed in parallel at the top of the second tower to condense the product at a pressure and temperature of 2.8 barg and 83°C. The feed introduced at tray 27 has a maximum feed rate of 14.5 ton/h and the main distillate component in the feed varies from 50 to 75% (by mass). The column operates at an average reflux ratio of 2.3 (mass), yielding 9 ton/h of distillate product.

## Capacity reduction problem

During the startup of the column after a plant turnaround in December 2019, the steam consumption of the thermosiphon reboiler suddenly dropped. In the meantime, higher water concentrations were observed in the feed and distillate samples. The first assumption about this — that the cooling water could have entered the process upstream of the column during the turnaround — was proven wrong when the water concentration in the feed subsequently dropped. However, the water concentration in the distillate did not decrease.

A ruptured tube in the thermosiphon reboiler (W48) was presumed to be the reason for the higher water concentration in the distillate. After draining the column and drying it with nitrogen, the redundant thermosiphon reboiler (W49) was taken into operation. The water concentration in the distillate decreased, and at the normal feed rate of 12 ton/h, product specifications were met. However, when the capacity was increased to a feed rate of 14 ton/h, the products no longer met specifications.

Whatever the cause, separation efficiency of the column K11/K12 decreased after the turnaround. Temperature surveys and field tests were conducted. The column data were matched to the data prior to the turnaround. The feed flow, overhead pressure and concentration profiles of columns before and after the turnaround are plotted in Figures 2 and 3. The specification limits of C2 of the product column K11/K12 and C1 of the downstream column K13 are indicated, along with the intervals of the off-specification product C2 and C1, corresponding to feed flow rates in 2019 and 2020.

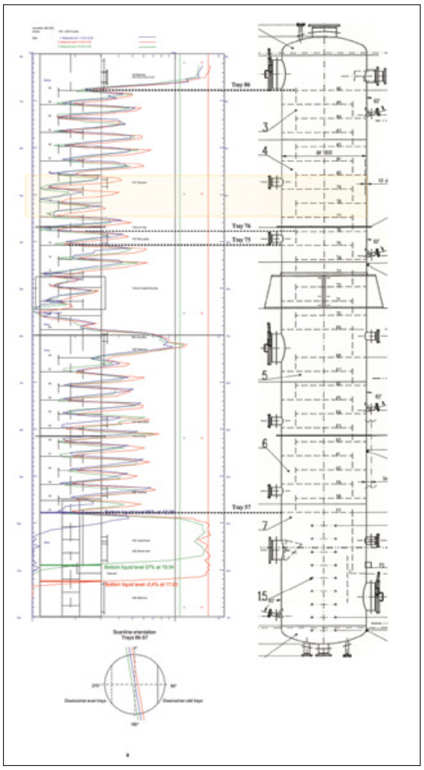
**FIGURE 4.** The gamma scan results (left) are shown next to the column diagram (right)

**FIGURE 5.** Photos from the column inspection showed contaminated trays (76 to 86; left photo) and clean trays (57 to 75; right photo)

The comparison shows that at above 14 ton/h, the distillate of the product column K11/K12 and the distillate of the downstream column K13 failed to meet specifications. The data analysis validates the finding that the separation efficiency of the column dropped after the reboiler leakage. Maximum feed rates of 14.5 ton/h and above were no longer feasible. Interestingly, the overhead pressure of the first tower K11 fluctuated significantly in contrast to the overhead pressure of the second tower K12 (see Figure 3). In addition, sudden temperature drops of the reflux and distillate streams at the top of the column indicated flooding in the condensation system.

The data reconciliation and temperature surveys led to the assessment that the reason for the capacity reduction could either be that the reflux piping was blocked, or that damaged trays in the second tower K12 led to flooding. Therefore, it was decided to carry out gamma scanning of the second tower K12 to identify the reason behind the capacity reduction.

## Gamma-scan troubleshooting

Gamma scanning of tower K12 was performed by the company IBE Ingenieurbüro Esper GmbH (Grünstadt, Germany; www.ide-engineering.com). Three scans of the active areas of trays 57 to 86 at a feed rate of 12 ton/h for different liquid levels in the column sump were performed. The results are shown next to the tower drawing in Figure 4. A baseline scan of the tower was not available for a comparative analysis.

The peaks of all 30 trays can be clearly seen, indicating that all trays are in place. The radiation intensity is low for trays 70 to 73 because the radiation gets absorbed by the column support ring. One of the findings during the gamma scanning was that of an incorrect installation of the liquid-level measurement in the column sump. Above 40% level indication, the liquid level is already above the vapor inlet. Increasing the liquid level results in higher liquid loads on the trays due to the liquid entrainment by the vapor inlet.

The main conclusion of the gamma scanning was that tower K12 was completely flooded. The vapor line (VL) on the right side of the radiation diagram is only touched on the top of the column. Lowering the liquid level in the column sump has a noticeable impact. The radiation intensity on all trays increased after lowering the liquid level. Nevertheless, the column is still flooded, even after lowering the liquid level below the vapor inlet.

It is important to note that trays 77 to 79 show high radiation absorption, especially at higher liquid levels in the column sump. In the sections below, it will be explained why these trays are highlighted. To summarize, the capacity reduction caused by flooding is confirmed by the gamma scanning, but the reason for the flooding is not clearly understood. To progress with the investigation, it was decided to combine the field tests and gamma scanning results with a hydraulic rating [*3, 4*].

## Hydraulic rating

Hydraulic rating was performed by Siemens AG (Frankfurt, Germany; www.siemens.com) with the in-

**TABLE 1. HYDRAULIC RATING OF BALLAST AND VARIOFLEX TRAYS**

| | | | | | | |
|---|---|---|---|---|---|---|
| Column diameter, mm | 1,800 | | | | | |
| Tray type | Ballast (float valve) | | | | Varioflex (caged valve) | |
| Valve type | V-1 and V-1X | | | | VV16 – 3L20 | |
| Section | Stripping | | Rectification | | | |
| | #1 – #26 | | #28 – #56 | | #57 – #86 | |
| Number of passes | 1 | | 1 | | 1 | |
| Tray spacing, mm | 300 | | 250 | | 300 | |
| Weir height, mm | 59 | | 59 | | 59 | |
| DC type | Straight | | Straight | | Straight | |
| DC clearance, mm | 46 | | 46 | | 46 | |
| DC width, top/bot, mm | 284 | | 284 | | 287 | |
| DC area, top/bot, $m^2$ | 0.25 | | 0.25 | | 0.26 | |
| Active area[1], $m^2$ | 1.46 | | 1.46 | | 1.51 | |
| | | | | | | |
| Tray number | #1 | | #55 | | #86 | |
| Feed rate, ton/h | 12 | 14 | 12 | 14 | 12 | 14 |
| | | | | | | |
| F-Factor[2], $Pa^{0.5}$ | 1.66 | 1.93 | 1.48 | 1.73 | 1.47 | 1.71 |
| DC backup flood (Glitsch), % | 44 | 46 | 45 | 47 | 38 | 42 |
| Jet flood (Fair), % | 59 | 68 | 54 | 63 | - | - |
| Entrainment (Fair), - | 0.012 | 0.026 | 0.039 | 0.086 | 0.007 | 0.013 |
| Pressure drop, mbar/tray | 9.2 | 9.8 | 7.6 | 8 | 7.3 | 8.5 |

*Notes:* *1. Superficial area minus the sum of DC top, DC seal and inactive areas.*
*2. Based on tray active area.*

house program KOBO4. The stage profiles (vapor and liquid rates) for the KOBO4 program were generated using a rigorous column model (RadFrac) in AspenPlus. The simulation parameters and distillate product specifications of the distillation column and reboiler were matched against plant data at unflooded conditions before the turnaround.

The results of the hydraulic rating are shown in Table 1, which shows a stripping section and rectification section consisting of different sets of valves. Trays 1, 55 and 86 had maximum vapor and liquid loads, and the results for these trays are listed corresponding to feed rates of 12 and 14 ton/h.

Ballast trays in the stripping section at maximum feed rate are near the upper operating limit. According to Glitsch's criterion [*5*], the downcomer backup flood should be below 50% for moderate gas densities between 16 and 48 $kg/m^3$, and the pressure drop of almost 10 mbar per tray is the upper limit for these types of trays.

Ballast trays in the lower part of the rectification section at maximum feed rate exhibit the same trend with respect to the downcomer backup flood, but due to lower gas densities (<16 $kg/m^3$) in this section, the allowable limit of Glitsch's criterion is 60%. Further, the fractional entrainment (moles entrained liquid per moles gross liquid downflow), according to Fair's correlation [*6*], is almost at the upper recommended limit of 0.1 (due to the lower tray spacing). This indicates an operating point close to the upper limit in this section, but the trays were still operable at maximum capacity before the turnaround.

Varioflex trays in the upper part of the rectification section were employed for higher turndown ratio, a 20-mm orifice in the valve plate offers this special capability. The gamma scans showed that these trays were flooded, but the evaluation shows otherwise and they are not causing a bottleneck. The F-Factor of less than 2 $Pa^{0.5}$, equivalent airflow per valve of less than 80 $m^3/h$, and the fractional entrainment values of around 0.01 are the important criteria to predict whether the trays approach a limit. In addition, the downcomer backup flood was well within the limits, not exceeding 60%, according to Glitsch's criterion, which, along with the pressure drop of 8.5 mbar per tray, clearly indicate that there is no flooding in the rectification section. This contradicts the results of the gamma scans and field test observations.

The hydraulic rating leads to only one conclusion: severe fouling in the upper part of the rectification section (second tower K12). This is a plausible reason for the flooding can explain the significant reduction in column capacity.

## Column inspection

During the turnaround in 2020, the tower field service team of Sulzer Chemtech GmbH (Winterthur, Switzerland; www.sulzer.com) was assigned to inspect and restore the second tower K12. The manways were opened and all trays were inspected. The pictures from the inspection are shown in Figure 5. Interestingly, trays 76 to 86 were highly contaminated, but the trays below, from 57 to 75 were clean. This also corresponds to the trays highlighted in the gamma scanning radiation diagram (see Figure 4).

A careful examination of the contamination has shown that it is the inorganic compound ferrous chloride (iron (II) chloride; $FeCl_2$). This hygroscopic material was formed during the reboiler leakage when water entered the column. Once chlorinated hydrocarbons come into contact with water, hydrogen chloride gas is formed. Hydrogen chloride reacts with carbon steel of the column shell and internals to form ferrous chloride. This compound is highly soluble in water and will therefore be accumulated at the top of the column, the only outlet for the water (as an azeotropic mixture) [*7*]. After the reboiler was replaced, the water concentration dropped and the remaining ferrous chloride in the column precipitated, because it is insoluble in nonpolar chlorinated hydrocarbons [*8*].

This phenomenon is the reason why severe fouling is observed on the top 10 trays of the column, whereas the rest of the column trays were completely clean. The contamination even blocked some orifices of

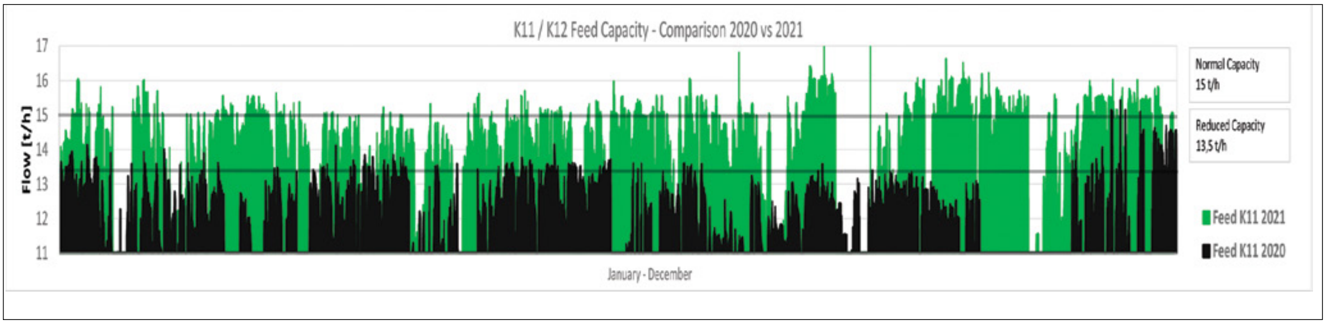


**FIGURE 6.** The column feed rates for 2020 (black lines) are compared to those for 2021 (green lines)

the caged valves and due to this reason, this section cannot be operated at higher gas loads. Interestingly, the gamma scans did indicate this area (trays 77 to 79). The contaminated trays were disassembled, cleaned with water, and then reassembled. Finally, the column was restarted after repositioning the level measurements in the sump of the second tower and increasing the diameter of the reflux piping.

The effects of the action can be seen in Figure 6, where feed rates to the column in the year 2020 are compared to those for 2021. In 2020 (dark peaks), the reduced capacity lies below the feed rate of 14 ton/h. After the turnaround, in the fourth quarter of 2020, an immediate improvement can be seen from the cleaning of contaminated trays, enabling maximum feed rates of 14.5 ton/h and above (green peaks).

## Concluding remarks

The combined efforts of field tests, gamma scanning and hydraulic rating led to the identification of a plausible reason for the capacity reduction — fouling of the trays. However, the fouling mechanism was only clearly understood during tower inspection, which revealed a very interesting phenomenon. In the end, the column capacity was able to be restored. It is pertinent to pay attention to the occurrences of steam leakages inside columns, and particularly those handling chlorinated hydrocarbons, where water entry can lead to capacity reduction and malfunction of columns. Luckily water, which caused the fouling, could also solve the problem by simple cleaning of the trays. ■

*Edited by Scott Jenkins*


## Acknowledgements

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All graphs and images in the article appear courtesy of Nobian GmbH.


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# Entrainment Flooding and Weeping Velocities

Weeping and flooding phenomena set the vapor velocity in industrial distillation columns. Presented here are procedures for calculating flooding and weeping velocities in a four-pass sieve-tray column

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Aramco

In industrial distillation, the term "weeping" is primarily used when the liquid in sieve-tray columns starts leaking through the holes or perforations as a result of insufficient counter-current vapor flow. Weeping is undesirable because the liquid should flow across the tray and through the downcomer. This sets the lower limit of vapor velocity for sieve-tray column operation (see box, Definitions). Conversely, the term "flooding" is used in sieve-tray columns where the excessive liquid build-up in the column leads to flooding condition. This is because the liquid cannot move down due to high vapor velocity. This sets the upper limit of vapor velocity for sieve-tray column operation. This article presents the procedure for calculating both flooding and weeping velocities, using both SI (International System of Units) and English Imperial System units.

## Four-pass sieve-tray columns

The most common types of gas-liquid mass-transfer operations are distillation and gas absorption, and the most common types of contactors used for distillation or gas absorption are packing or tray columns. The different types of packed and tray columns are shown in Figure 1.

As the liquid load increases, the number of passes can be increased from single-pass to as high as four- or six-pass trays. Three-pass trays are generally avoided due to the lack of symmetry of the trays. This article discusses only four-pass sieve-tray columns.

All four-pass sieve trays have three types of downcomers (Figure 2). Side downcomers are formed by a column wall and a downcomer panel. The center downcomer is located at the tower centerline and is formed between two downcomer panels offset from the centerline. Two side downcomers and a center downcomer are located on alternating trays, either on all odd-numbered or on all even-numbered trays. The third type of downcomers are off-center downcomers (OCDCs). The OCDC is located between the side and center downcomers on alternating trays — between the trays containing the side and center downcomers.

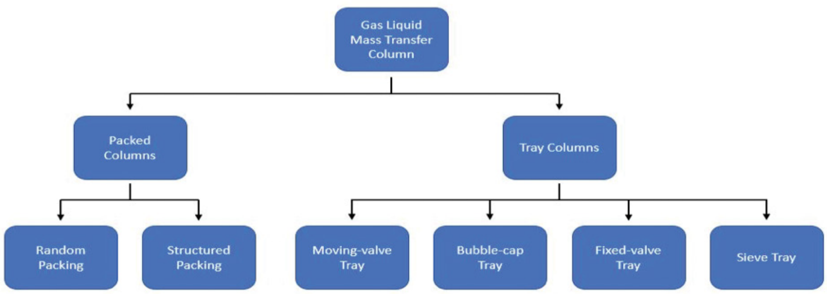


**FIGURE 1.** Different types of trayed and packed columns are categorized here

## Operating range

Satisfactory operation for this type of column is only achieved over a limited range of vapor and liquid flowrates. A typical performance diagram for a sieve plate is shown in Figure 3 [2].

The upper limit to vapor flow is set by the condition of flooding, while the lower limit of the vapor flow is set by the condition of weeping.

### DEFINITIONS

***Four-pass sieve-tray column.*** In a four-pass sieve-tray distillation column, every alternate tray is similar. A typical four-pass sieve tray will have two side downcomers and one center downcomer, while the next tray will have two off-center downcomers. The next tray will again have two side downcomers and a center downcomer. This cycle continues through the height of the column.

***Column cross-sectional area, $A_T$.*** The area of the column calculated based on the diameter of the tower.

***Total hole area, $A_H$.*** Total area of all the active holes/perforations on the sieve tray

***Net area, $A_N$.*** Column cross-sectional area minus the total downcomer area of the sieve tray

***Active/bubbling area, $A_B$.*** Column cross-sectional area minus the total downcomer area and the downcomer seal area (of the upper tray).

***Fractional hole area, $A_f$.*** The ratio between the total hole area and the active/bubbling area ($A_H/A_B$).

***Downcomer area, $A_{DC}$.*** Area occupied by the downcomers. Area of the side downcomers formed by the column wall and the downcomer panel can be calculated using Table 4 in the Koch-Glitsch Tray Design Manual Bulletin 4900 [1]

***Outlet weir height, $h_w$.*** Outlet weir height maintains a liquid level on the tray and should be high enough to provide sufficient contact between liquid and vapors without excessive pressure drop.

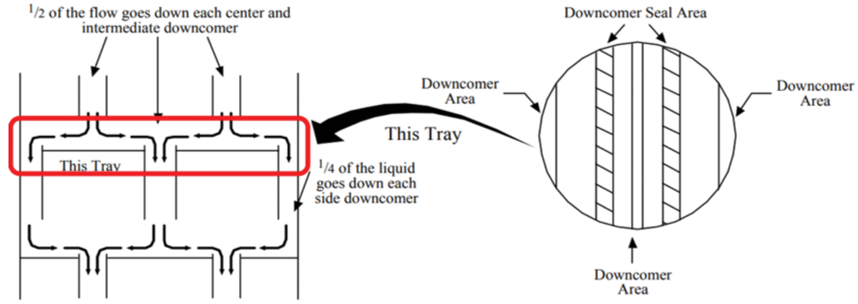


**FIGURE 2.** The diagram shows the arrangement of a typical four-pass sieve tray column, with path flow on each tray

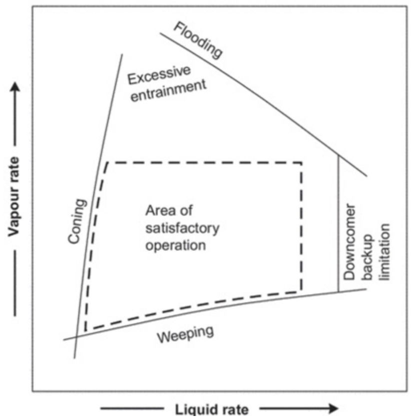


**FIGURE 3.** On this graph, a typical performance diagram for a sieve plate is shown, with the area of operation between flooding and weeping

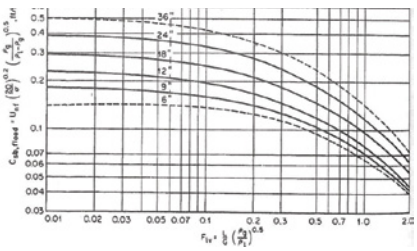


**FIGURE 4.** The C-factor can be estimated from this graph from Ref. 10

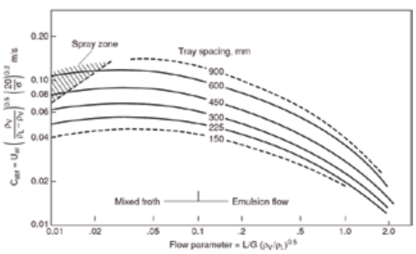


**FIGURE 5.** The C-factor can be estimated from this graph from Ref. 4

## Entrainment and flooding

Two methods outlined below can be used for calculating flooding velocity.

***Fair's method.*** The method by J.R. Fair [3] is described as follows: Calculate flow parameter $F_{LV}$, Equation (1).

$$F_{LV} = \frac{L}{V}\sqrt{\frac{\rho_V}{\rho_L}} \tag{1}$$

For multi-pass trays, *L/V* ratio should be divided by the number of passes, which in this case is four [4].

Estimate Souder's & Brown [5] coefficient $C_{SB}$ (also known as C-factor), using the graphs in Figures 4 and 5. Alternatively, Souder's & Brown coefficient ($C_{SB}$) can be calculated empirically using Equation (2) for SI units [6].

$$C_{SB} = 0.0105 + \left[0.1496 \times S^{0.755} \times e^{\left(-1.463 \times F_{LV}{}^{0.842}\right)}\right] \tag{2}$$

or Equation (3) for English units [7]:

$$C_{SB} = \frac{0.26S - 0.029S^2}{\left[1 + 6F_{LV}{}^2 S^{0.7498}\right]^{0.5}} \tag{3}$$

Flood-point vapor velocity can be estimated using Equation (4).

$$u_{flood} = C_{SB}\left(\frac{\sigma}{20}\right)^{0.2}\sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \tag{4}$$

***Kister and Haas method.*** Kister and Haas [8] developed the correlation to calculate Souder's & Brown coefficient ($C_{SB}$) for sieve-tray flood point given in Equations (5) (English units) [10] and (6) (SI units) [4].

$$C_{SB} = 0.144\left[\frac{d_H{}^2\sigma}{\rho_L}\right]^{0.125}\left(\frac{\rho_V}{\rho_L}\right)^{0.1}\left(\frac{S}{h_{ct}}\right)^{0.5} \tag{5}$$

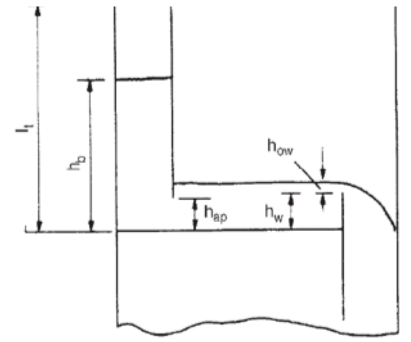


**FIGURE 6.** This diagram shows the liquid height over the weir, from Ref. 2

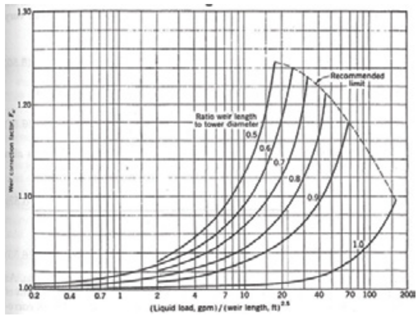


**FIGURE 7.** The correction factor from Equation (11) can be estimated from this graph from Ref. 10

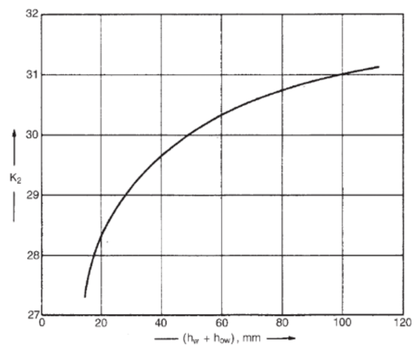


**FIGURE 8.** The coefficient $K_2$ from Equation (13) can be estimated using this graph from Ref. 2

where:
$S$ = tray spacing, in.
$d_H$ = hole diameter, in.
$h_{ct}$ = clear liquid height at froth-to-spray regime, in.

$$C_{SB} = 0.0277\left[\frac{{d_H}^2\sigma}{\rho_L}\right]^{0.125}\left(\frac{\rho_V}{\rho_L}\right)^{0.1}\left(\frac{S}{h_{ct}}\right)^{0.5} \quad (6)$$

where:
$S$ = tray spacing, mm
$d_H$ = hole diameter, mm
$h_{ct}$ = clear liquid height at froth-to-spray regime, mm

Clear liquid height at the froth-to-spray regime transition, corrected for the effect of weir height on spray regime entrainment can be calculated using Equation (7) [8].

$$h_{ct} = \frac{h_{ct,\,H_2O}}{1{+}0.00262h_W}\left(\frac{996}{\rho_L}\right)^{0.5(1-n)} \quad (7)$$

where:
$h_{ct}$ = clear liquid height at froth-to-spray regime, mm
$h_{ct,\,H2O}$ = clear liquid height at froth-to-spray regime for air-water system, mm
$h_W$ = outlet weir height, mm
$n = 0.00091\ (d_H/A_f)$

For an air-water system, the clear liquid height can be calculated by using the modified Jeronimo and Sawistowski Correlation (Equation (8)):

$$h_{ct,\,H_2O} = \frac{0.4974{A_f}^{-0.791}d_H^{0.833}}{1{+}0.013{Q_L}^{-0.59}A_f^{-1.79}} \quad (8)$$

Similarly, for English Units, the equation is shown in Equation (9) [10].

$$h_{ct} = \frac{h_{ct,\,H_2O}}{1{+}0.0665h_W}\left(\frac{62.2}{\rho_L}\right)^{0.5(1-n)} \quad (9)$$

where:
$h_W$ = outlet weir height, in.
$n = 0.0231\ (d_H/A_f)$
and:

$$h_{ct,\,H_2O} = \frac{0.29{A_f}^{-0.791}d_H^{0.833}}{1 + 0.0036{Q_L}^{-0.59}A_f^{-1.79}}$$

Flood-point vapor velocity can then be calculated as follows:

$$u_{flood} = C_{SB}\left(\frac{\sigma}{20}\right)^{0.2}\sqrt{\frac{\rho_L-\rho_V}{\rho_V}} \quad (10)$$

## Weeping

Liquid height over the weir $h_{ow}$ is calculated using the corrected Francis formula, as shown in Equation (11) (English units) and Equation (12) (SI units):

$$h_{ow} = 0.48 \times F_W(Q_L^{2/3}) \quad (11)$$

### NOMENCLATURE

| | |
|---|---|
| $A_f$ | Fractional hole, $A_H/A_B$ |
| $A_H$ | Total hole area, ft$^2$ or m$^2$ |
| $A_B$ | Active/bubbling area, ft$^2$ or m$^2$ |
| $C_{SB}$ | Souder's and Brown coefficient, ft/s or m/s |
| $d_H$ | Hole diameter, in. or mm |
| $F_{LV}$ | Flow parameter |
| $F_w$ | Correction factor |
| $h_{ct}$ | Clear liquid height at froth-to-spray regime, in. or mm |
| $h_{ct,\,H2O}$ | Clear liquid height at froth-to-spray regime for air-water system, (in. or mm) |
| $h_{ow}$ | Liquid height over the weir, in. or mm |
| $h_W$ | Outlet weir height, mm |
| $L$ | Liquid flowrate, lb/hr or kg/h |
| $Q_L$ | Liquid Flux, (gal/min per in. or m$^3$/h per m |
| $S$ | Tray spacing, m or ft |
| $u_{flood}$ | Vapor velocity at flood, (ft/s or m/s) |
| $u_{weeping}$ | Weeping velocity, ft/s or m/s |
| $\rho_V$ | Gas or vapor density, lb/ft$^3$ or kg/m$^3$ |
| $\rho_L$ | Liquid density, lb/ft$^3$ or kg/m$^3$ |
| $\sigma$ | Surface tension, dyne/cm or mN/m |

where:
$h_{ow}$ = liquid height over the weir, in.
$F_W$ = correction factor

$$h_{ow} = 664 \times F_W(Q_L^{2/3}) \quad (12)$$

where:
$h_{ow}$ = liquid height over the weir, mm
$F_W$ = correction factor

The correction factor $F_W$ in Equations (11) and (12) can be estimated using the graph in Figure 7 [10].

Weeping velocity can be calculated using the Eduljee Correlation [9, 11], in either SI units (Equation (13)) or English units (Equation (14)).

$$u_{weeping} = \frac{[K_2{-}0.90(25.4{-}d_H)]}{{\rho_V}^{0.5}} \quad (13)$$

where:
$u_{weeping}$ = vapor velocity at weep point, m/s
$d_H$ = hole diameter, mm

$$u_{weeping} = \frac{[K_2{-}18.8(1{-}d_H)]}{{\rho_V}^{0.5}} \quad (14)$$

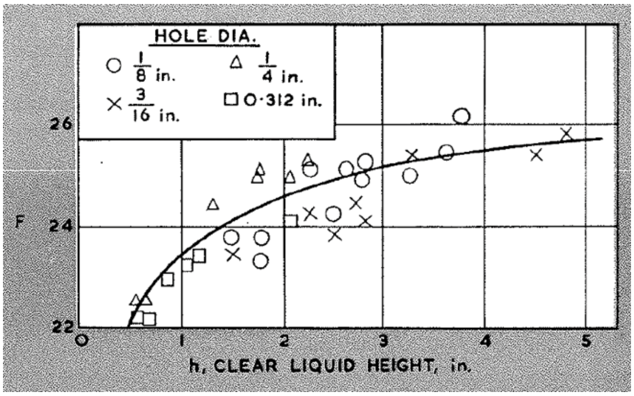


**FIGURE 9.** This graph from Ref. 9 can help estimate the coefficient $K_2$ from Equation (14)

where:

$u_{weeping}$ = vapor velocity at weep point, ft/s

$d_H$ = hole diameter, in.

The coefficient $K_2$ in the above correlations can be estimated using the graphs in Figures 8 and 9 [*2, 9*]. ■

*Edited by Scott Jenkins*

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# Safeguarding the Hydrogen Economy: A Focus on Leak Detection and Mitigation

## The use of fixed gas detectors can play a crucial role in mitigating the environmental impact of hydrogen leakage and help protect workers in the hydrogen value chain

**Mark Heuchert and Ronak Patel**
Dräger North America

### IN BRIEF



Governments, industry sectors and companies seeking sustainable energy sources to reduce greenhouse gas (GHG) emissions are increasingly turning to hydrogen. In a recent survey of 500 global energy and utilities-sector executives and 360 executives from end-user sectors (including heavy transportation, aviation, maritime transport, steel, chemicals and petroleum refining), 64% said they plan to invest in low-carbon hydrogen initiatives by 2030, and 9 out of 10 plan to do so by 2050 [*1*].

"Low-carbon hydrogen will play a key role in the decarbonization of several industries whose emissions are difficult to abate, such as basic chemicals, aviation, steel production, shipping and long-haul road transportation," stated Boston Consulting Group (BSG), authors of the March 2023 Building the Green Hydrogen Economy report [*2*].

On the surface, hydrogen appears to be an ideal energy source to help pave the path to a more sustainable future. However, since $H_2$ is the smallest molecule in existence, it can easily pass through and embrittle materials and sealings. Therefore, potential for leakage presents significant challenges and risks throughout the hydrogen value chain.

While hydrogen emits no carbon dioxide when burned or used in a fuel cell, its leakage into the atmosphere has an indirect impact on global warming by extending the lifetime of GHGs, such as methane, ozone and water vapor, resulting in indirect warming [*3*, *4*].

Global energy experts are calling for increased research and development to "improve hydrogen leakage detection, prevention and mitigation," noting how "hydrogen sensors must be able to detect leakage at much lower detection thresholds than those existing and among various types of applications [*3*]."

This technology exists today in the form of fixed gas detectors that can monitor for small leaks before they become more significant, and initiate automatic ventilation, engine room shutdowns and other actions as required for larger releases and accidents (Figure 1).

When used throughout the hydrogen value chain, from production and delivery to storage, tank maintenance and power generation, fixed gas detection can help mitigate the potential environmental impact of unintentional hydrogen leakage and help protect workers who are enabling the steps in the value chain.

### Current and future $H_2$ applications

The most common industrial uses of hydrogen today are for chemical feedstocks, petroleum refining and fertilizer production. More than 90% of the world's hydrogen is used for three industrial applications: by petroleum refineries to lower sulfur content in diesel; to produce methanol used by fuel blenders; and make ammonia for fertilizers and chemicals [*5*]. A small percentage of hydrogen is consumed directly in steel production [*6*].

There are four main types of hydrogen production [*3*, *7*, *8*], as follows:

1. Brown or black hydrogen produced from coal. It is the most environmentally damaging form of hydrogen production because both the $CO_2$ and CO generated during the process are not recaptured, creating significant air emissions
2. Gray hydrogen produced from natural gas using a process known as steam reforming, which releases carbon emissions. It typically generates a somewhat smaller amount of emissions than black or brown hydrogen
3. Blue hydrogen produced using the same


**FIGURE 1.** Because of hydrogen's unique physical properties, gas detection is paramount in preventing leakage, losses and other serious issues

process as gray hydrogen, but is augmented with carbon capture, utilization and storage (CCUS) technology to mitigate emissions. It is sometimes referred to as "carbon neutral, as the emissions are not dispersed in the atmosphere," but a more accurate description is "low-carbon" because around 10–20% of the generated carbon cannot typically be captured

4. Green hydrogen produced using renewable energy, usually through water electrolysis. This results in no emissions

Gray hydrogen is the most common form of hydrogen production today (over 90%) but there has been growing interest and significant investments in low-carbon and emissions-free hydrogen production across the globe [*9*]. The Center on Global Energy Policy predicts blue and green hydrogen to comprise 97% of the total supply by 2050 [*3*].

Some targeted use cases for clean hydrogen and recently announced initiatives are described in the following sections.

***Steel production.*** The steel industry produces more $CO_2$ than any other heavy industry, comprising about 8% of total global GHG emissions [*10*], making it a prime target for clean hydrogen-based initiatives. In April 2023, India's largest steelmaker, Tata Steel, announced that it had begun a trial of injecting hydrogen gas at its blast furnace to cut carbon emissions [*11*].

***Fertilizer production.*** The production and use of nitrogen fertilizers accounts for up to 5% of total GHG emissions [*12*]. Research published in 2023 found that changing the source of hydrogen for ammonia production from steam reforming (gray hydrogen) to water electrolysis (green hydrogen) could reduce 75% of production emissions by 2050 [*12*]. Fertilizer company Yara, utilities company Engie and investment and trading company Mitsui & Co. are collaborating on the Yuri Renewable Hydrogen to Ammonia Project, scheduled for completion in December 2027 [*13*].

***Petroleum refining.*** The refining sector is a major energy user and contributes to approximately 4% of GHG emissions. It is the third-highest emitter amongst industrial sectors (excluding energy production), making it another prime target for clean hydrogen adoption [*14*]. In July 2022, Irving Oil announced that it was expanding its green hydrogen capacity with investment in 5-megawatt hydrogen electrolyzer [*15*].

## Trouble spots for $H_2$ leakage

While low-emission and emissions-free hydrogen production has significant potential to reduce carbon emissions and support global sustainability efforts, hydrogen leakage during production, transport, storage and end use could negate the benefits and potentially result in enduring climate impacts [*16*]. Because hydrogen production and use are limited today, and the infrastructure does not yet exist to broaden its use to the levels anticipated by 2050, there is uncertainty around the risk for hydrogen leakage throughout the value chain. Researchers have relied on estimates based on current usage, and projections based on the value chain of other gases like natural gas.

## Production

When hydrogen is produced via electrolysis, the most significant mechanism for leakage is operational purging as part of the purification process, with leakage as high as 10%. During CCUS-enabled hydrogen production, similarly to electrolysis, hydrogen can potentially be released from leakage or purging. Even if waste hydrogen is "sent to flare rather than vented to atmosphere," there will be residual hydrogen emissions, estimated at between 0 and 0.5% of the hydrogen produced [*17*].

Hydrogen leakage during production seems to vary by production method. Leakage during gray hydrogen production (via steam reforming) is estimated at less than 1%. Leakage during blue hydrogen production (with CCUS technology) is estimated to be approximately 1.5% because of the "added complexities of its production system [*3*]."

Because green hydrogen production is very limited today, researchers struggle to estimate its leakage, but it is an important research topic, given predictions that its use will expand. Looking at studies on green hydrogen "losses," which means measuring the "difference between the theoretical, calculated quantity of hydrogen that is supposed to be produced and the amount that is actually measured," the total loss could be as high as 4% [*3*].

## Delivery, transport and storage

While most hydrogen consumed today is obtained locally, it can be transported to terminals via pipelines, trucks, trains or ships. Hydrogen is stored in liquid (cryogenic) or gaseous (compressed) phases in terminals until it is distributed to end-users at petroleum refineries, chemical plants and so on.

According to the Center on Global Energy Policy, "pipelines, including both dedicated hydrogen pipelines and natural gas blending systems, are the most important systems for hydrogen delivery" and "in and of themselves, these systems demonstrate a low risk of leakage [*3*]."

Studies published in recent years have found "roughly 0.4% leakage for hydrogen simply passing through a pipeline [*18*]." But this does not consider the full hydrogen delivery systems that will be required to support the future hydrogen economy, including storage


**FIGURE 2. Gas detection is crucial to ensure reliable explosion prevention in hydrogen production and handling applications**

facilities, which could experience mechanical loss. Researchers estimate a 2% lifecycle loss of hydrogen from integrated transportation and storage systems [*3*].

The delivery of hydrogen to fueling systems via trucks is "leakier," according to the Center on Global Energy Policy, with an estimated 5% average leakage for truck transport and storage systems. Leakage of hydrogen for particularly small facilities (<100 kg/d) is estimated to be above 20%, and average-sized fueling stations (several hundreds to several thousands of kilograms per day), between 3 and 6% [*3*].

## End use

The end users for hydrogen are expected to expand with greater investment in the production of blue and green hydrogen. The challenge is that "end-use leakage risks are the least understood especially in terms of future hydrogen end uses that do not exist today [*3*]." Described below are current and anticipated use cases and estimated risks for leakage.

***Electricity generation.*** The process of converting hydrogen to power based on gas-turbine technology has around 3% hydrogen leakage [*3*].

***Fuel cells (surface and aviation transport).*** Fuel cells emit "a similar amount of hydrogen compared to electrolyzers and, when incorporated into transport applications, will also emit hydrogen from the compressed storage [*17*]." In a study that assumed "road transport leakage is similar to hydrogen storage tank leakage during delivery, with the exception of potential boil-off loss during charging," researchers estimated road transport leakage at 2.3% [*3*].

***Hydrogen refueling stations.*** Here, the main emissions are from the compression of hydrogen and the short-term storage of compressed hydrogen prior to injection into vehicles. Experts predict these emissions "should be relatively low (at 50% confidence) but there are some uncertainties that push up the upper limit (99% confidence) [*17*]."

***Industry (to decarbonize industrial processes such as steel and chemicals).*** While it has not been "possible to predict the emissions from industry at this stage and this will require further consideration," researchers assume an "emission of between 0 and 0.5% of the hydrogen used [*17*]."

## Risks to the environment

New research from Princeton University and the National Oceanic and Atmospheric Association (NOAA) found "a leaky hydrogen economy could cause near-term environmental harm by increasing the amount of methane in the atmosphere. The risk for harm is compounded for hydrogen production methods using methane as an input, highlighting the critical need to manage and minimize emissions from hydrogen production [*16*]."

As the Center on Global Energy Policy pointed out in its report, the more hydrogen produced, the more leakage into the atmosphere if mitigation measures are not put in place. The estimated 2.7% economy-wide leakage in 2020 could jump to 5.6% leakage in 2050 based on hydrogen production milestones (528 million metric tons by 2050) outlined in the International Energy Agency (IEA) net-zero scenario [*3*].

The Princeton and NOAA researchers have established the following leakage thresholds for green and blue hydrogen in Ref. 16.

***Green hydrogen: critical threshold for emissions is around 9%.*** "If more than 9% of the green hydrogen produced leaks into the atmosphere — whether that be at the point of production, sometime during transport, or anywhere else along the value chain — atmospheric methane would increase over the next few decades, canceling out some of the climate benefits of switching away from fossil fuels."

***Blue hydrogen: critical threshold for emissions is around 4.5%.*** "Because methane itself is the primary input for the process of methane reforming, blue hydrogen producers have to consider direct methane leakage in addition to hydrogen leakage. For example, the researchers found that even with a methane leakage rate as low as 0.5%, hydrogen leakages would have to be kept under around 4.5% to avoid increasing atmospheric methane concentrations."

## Risks to workers

While hydrogen itself is not toxic and does not impose major new risks compared to other gases, leakage can impact the safety of people involved in tasks along the hydrogen value chain, from production to use. Below are some of hydrogen's characteristics that employers and workers must take into consideration when building a safety infrastructure.

***Permeation.*** Hydrogen can easily permeate materials and in some cases embrittle them. For this reason, stainless steel and composite materials are typically used for storage tanks.

***Leakage.*** Owing to its small molecules and low viscosity, hydrogen can leak from pipelines and other structures more easily than denser gases. In fact, when it leaks from a pipe at sufficiently high pressure, hydrogen can even self-ignite. As well as with pipelines engineered to hydrogen-ready specifications, regular inspection is imperative to detect leak points at joints and along pipelines.

***Explosion.*** Unlike actual explosives, pure hydrogen cannot explode. The risk comes when it hits the air. For hydrogen to cause an explosion,

oxygen needs to be present. But if hydrogen is allowed to escape, even a static spark from clothing would be enough to set off an explosion.

***Invisible flame.*** Hydrogen burns with a very pale flame that is invisible in daylight. Because it emits little of the infrared radiation that humans perceive as heat, it cannot be sensed as heat. The hydrogen flame does however emit substantial ultraviolet radiation.

***Odorless and colorless.*** Hydrogen has no smell and no color, so it is undetectable for humans. With methane, this issue is mitigated by adding odorants, and research is in progress to determine whether this will also be possible with hydrogen.

## Gas detection requirements

Given its propensity for permeation and leaks, inability of humans to detect in their environments and risk for explosion, hydrogen must be continuously and reliably monitored throughout its value chain. The ability to detect small leaks can help organizations prevent the escape of large "fugitive emissions" into facilities and out into the atmosphere [*17*].

If systems are designed correctly, such very small leaks will not pose issues, because the amount of hydrogen gas released will typically be too small to create a flammable mixture with air. Risks (including asphyxiation or the creation of a flammable mixture) only arise when hydrogen gas accumulates in a confined area over time [*19*].

Due to the properties of hydrogen, explosion protection via early leak detection is key to ensuring plant and personal safety. Gas detection is regarded as the primary way to protect against explosion by preventing explosive atmospheres from building in the first place (Figure 2).

Organizations in the hydrogen value chain must engage in risk control, including deployment of gas measuring and warning systems, to comply with standards, codes and regulations. A few examples are outlined here.

***ISO 26142 Hydrogen Detection Apparatus – Stationary applications.*** This is an international standard that "defines the performance requirements and test methods of stationary hydrogen detection apparatus that is designed to measure and monitor hydrogen concentrations." It sets requirements "applicable to a product standard for hydrogen detection apparatus, such as precision, response time, stability, measuring range, selectivity and poisoning [*20*]."

***H-14: HYCO Plant Gas Leak Detection and Response Practices.*** This applies to plants producing large amounts of hydrogen and carbon monoxide. It covers methodologies for prevention of, detection of, and response to flammable and/or toxic gas leaks that occur within the fence line of these facilities, including typical leak detection technologies (for instance, personal monitoring, fixed monitoring, and specialized detectors) [*21*].

***UL 2075 Standard for Safety Gas and Vapor Detectors and Sensors.*** This applies to fixed, portable and transportable toxic and combustible gas and vapor detectors and sensors intended for use in ordinary (non-hazardous) locations for use in indoor or in unconditioned areas [*22*].

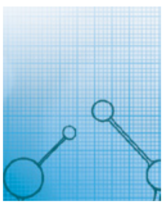

FIGURE 3. Some portable gas detectors can be configured for detecting hydrogen along with multiple other gases

## Fixed hydrogen gas detection

Fixed gas-detection systems provide instant alerts in the event of hazardous leaks or risks of combustion. Organizations can leverage several different hydrogen detection technologies to build efficient and effective protection layers.

***Catalytic bead sensor.*** This sensor type detects hydrogen below its lower explosive limit (100% LEL). With good long-term stability and fast response time, these devices are mainly used for continuous area monitoring of the ambient air.

***Flame detectors.*** This type of device detects hydrogen-based fires, which are barely visible to the human eye. Those with sensor technology and programming specially designed for hydrogen or its combustion product ($H_2O$) ensure rapid detection of the dangerous flames and, at the same time, very high immunity to false alarms, which, for example, multifunction devices cannot provide to the same extent.

***Ultrasonic gas-leak detection.*** Ultrasonic detectors "listen" to high-pressure leaks and can detect even small leaks very fast. They serve as early warning area monitors, responding earlier than conventional gas detectors because they register the sound of leaking gas instead of measuring the concentration of accumulated gas clouds.

***Electrochemical sensor (EC).*** These devices are a good choice when selective measurements of hydrogen on the parts-per-million (ppm) concentration level are required. They offer many advantages, such as fast response, high accuracy, great stability and a long service life. This technology is useful for point leak detection and personal air monitoring.

## Safe and effective detection

Hydrogen detection systems are only as effective as the planning that goes into them. The organization and its detection system technology partner should first conduct an on-site risk assessment to know exactly where to place sensors, how sensitive they must be and what happens in the event of an alarm. Fixed gas detectors with a modular design can be flexibly integrated into an existing infrastructure, combined with each other, and extended into a seamless safety network.

One key consideration during the risk assessment is determining where hydrogen will go in the event of a leak. Like ammonia and methane, hydrogen is less dense than air and forms gas pockets below indoor ceilings when leaking. The presence of hydrogen will not be perceived at ground level, even when dangerous amounts are accumulating beneath the ceiling. When hydrogen and methane are mixed, hydrogen can form gas pockets above methane. Hydrogen detectors are therefore typically placed at a higher level than methane detectors.

It is also important to note that CO sensors are cross-sensitive to hydrogen. If used near possible hydrogen exposure, CO sensors should be compensated for hydrogen so that cross-sensitivity and false alarms are reduced to a minimum.

An organization should work with its technology partner to incorporate fixed hydrogen detection devices into its broader alarm and emergency response network. Advanced technology, such as flame and gas mapping, help to develop suitable solutions for specific organizational needs.

## Digitalization in gas detection

As compliance requirements become stricter, organizations are mandated to maintain detailed records — for example, of measured gas values or alarms — to demonstrate adherence to safety standards. Manual, paper-based recording and tracking of data in the hydrogen value chain cannot support safety measures at the scale in which hydrogen use is predicted to grow.

In a bid to raise the efficiency of documentation tasks and make use of the large amount of data generated, organizations are turning to solutions with smart data analytics. Data captured by hydrogen detectors are processed in a single, automated workflow for record keeping, and turns raw data into valuable insights for operational safety.

Digital technologies will be essential to the hydrogen value chain, including for system surveillance, early detection of faults and leaks and continuous optimization of costs [*1*]. The digital records are more accurate and can be made available faster during audits. Predictions and improvements can also be derived from data patterns. Impending failures can be prevented before they occur, and leaks and defects can be detected before they lead to serious damage.

## Portable gas detection

Mobile hydrogen-detection devices serve as an adjunct to fixed hydrogen detection monitors. Small, robust and ergonomic, these devices are usually attached to a worker's clothing near the breathing area, but in a way as to not limit their movement. Portable gas detection instruments can be equipped with sensors to detect hydrogen alone or other gases as well — for instance, $O_2$, CO, $H_2S$, $NO_2$ and $SO_2$ (Figure 3).

As with the fixed hydrogen-detection monitors, mobile detection devices should feature the ability to wirelessly transmit measured data to a central gas detection system. That way, the organization has a central, digital repository of measured gas values, alarms and other data for analytics, documentation and reporting.

Hydrogen is increasingly being recognized as a key player in the transition towards a more sustainable future. Governments, industry sectors and companies are planning significant investments in low-carbon hydrogen initiatives to reduce emissions in industries that are difficult to decarbonize.

However, the potential for hydrogen leakage presents significant challenges and risks throughout the hydrogen value chain, indirectly impacting global warming. Therefore, there is a need for increased research and development to improve hydrogen leakage detection, prevention and mitigation. ■

*Edited by Mary Page Bailey*

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# Enhancing Communication in Engineering Teams

## Clear communication among team members is important for a successful engineering project. Tips for avoiding pitfalls are outlined here

Lars Gerull

In the fast-paced world of engineering, mastering communication and conflict resolution is essential for team success and project efficiency. Engineering teams often comprise individuals with diverse expertise and backgrounds, making clear communication vital for project success. Conflicts are inevitable, but if managed properly, they can turn into opportunities for growth and innovation.

Enhancing communication and conflict resolution in engineering teams is essential for fostering a productive and harmonious work environment. By promoting open communication, utilizing technology, addressing conflicts early and fostering team cohesion, engineering teams can improve their dynamics and project outcomes. Implementing these techniques not only enhances the efficiency and effectiveness of the team but also contributes to the personal and professional growth of its members.

Building a culture of open communication and effective conflict resolution requires ongoing effort and commitment from all team members. By prioritizing these aspects, engineering teams can create a more collaborative, innovative and resilient work environment that benefits everyone involved (Figure 1). This article explores practical strategies engineers can use to enhance communication and resolve conflicts, thereby improving team dynamics and project outcomes.

### Good communication matters

Effective communication is the backbone of successful engineering projects. It ensures everyone on the team is aligned, understands their roles, and can collaborate efficiently. Clear communication prevents misunderstandings that can lead to errors, extra work and delays. Moreover, it fosters teamwork and innovation that keeps projects on track by ensuring milestones and deadlines are met. When communication flows smoothly, it builds trust and fosters a collaborative environment where team members feel valued and heard. This, in turn, boosts morale and increases productivity. Conversely, poor communication can lead to misunderstandings, frustration, and conflicts, ultimately derailing projects and damaging relationships.


**FIGURE 1.** Building a culture of open communication and effective conflict resolution requires ongoing effort and commitment from all team members

### Common hurdles

Before diving into improvement strategies, it's crucial to recognize the common obstacles engineering teams face. Technical jargon can often confuse non-specialists. Cultural differences within diverse teams can create challenges due to varying communication styles and norms. Hierarchical structures may hinder open communication between different levels of the team. Additionally, with remote work becoming more prevalent, effective communication across locations and time zones can be difficult.

***Technical jargon.*** Engineering is filled with specialized language and technical terms. While this jargon is necessary for precise communication among experts, it can create barriers when communicating with non-specialists or team members from different disciplines. Overusing technical jargon can lead to misunderstandings and confusion, hindering effective collaboration.

***Cultural differences.*** In today's globalized world, engineering teams often consist of individuals from diverse cultural backgrounds. Different cultures have different communication styles, norms and expectations. What is considered polite and respectful in one culture may be perceived as rude or dismissive in another. These cultural differences can lead to misunderstandings and conflicts if not managed properly.

***Hierarchical structures.*** Many engineering teams operate within hierarchical organizational structures. While these structures can help maintain order and clarity of roles, they can also create barriers to open communication. Team members may feel hesitant to share their ideas or concerns with higher-ups, fearing retribution or dismissal. This can stifle innovation and prevent important issues from being addressed.

***Remote work.*** The increase in remote work has introduced new communication challenges. Team mem-

bers working from different locations and time zones can face difficulties in coordinating and collaborating effectively. Miscommunications are more likely to occur when face-to-face interactions are limited, and team members rely heavily on digital communication tools.

## Improving communication

Several techniques to boost communication in engineering teams are outlined here:

***Promote open communication.*** Creating a culture where team members feel comfortable sharing their thoughts, concerns and ideas is crucial. Team leaders should lead by example, being transparent and approachable. Creating safe spaces, such as regular meetings or forums, allows team members to speak freely without fear of judgment. Active listening, where leaders and team members show that everyone's input is valued and considered, is essential.

Encouraging open communication involves fostering an environment where feedback is welcomed and valued. Team members should feel confident that their ideas and concerns will be heard and addressed constructively. This can be achieved through regular team meetings, open-door policies and anonymous feedback channels.

***Use clear and simple language.*** To avoid misunderstandings and ensure everyone is on the same page, simplify technical jargon and use language that's easy for all team members, including non-specialists, to understand. Be specific in your instructions and feedback to eliminate ambiguity. Reiterating and summarizing key points during discussions ensures everyone grasps the topic.

Clear communication is about more than just using simple language — it's also about being concise and to the point. Avoiding unnecessary details and focusing on the main message helps ensure that the information is understood correctly. Visual aids, such as diagrams and flowcharts, can also enhance understanding, especially when explaining complex technical concepts.

***Leverage technology.*** Modern communication tools can bridge gaps and enhance clarity. Project management software like Asana, Trello and Jira keeps everyone updated on project progress. Communication platforms such as Slack, Microsoft Teams and Zoom facilitate real-time communication and collaboration. Document-sharing platforms like Google Drive or SharePoint ensure all team members have access to the latest project documents.

Using technology effectively involves selecting the right tools for your team's needs and ensuring that all team members are proficient in using them. Providing training and support for these tools can help maximize their benefits. Additionally, setting clear guidelines for digital communication, such as response times and preferred channels, can help streamline interactions and reduce misunderstandings.

***Foster cross-functional collaboration.*** Encouraging collaboration between different departments and specialties enhances team dynamics. Forming interdisciplinary teams with diverse expertise fosters innovation and problem-solving. Regular cross-functional meetings promote knowledge sharing and collaboration, helping to break down silos and improve overall team performance.

Cross-functional collaboration involves more than just bringing together team members from different departments; it also requires creating opportunities for them to interact and work together. This can be achieved through joint projects, workshops and team-building activities. Encouraging open dialog and mutual respect among team members from different disciplines helps create a more cohesive and collaborative team environment.

## Conflict resolution

Poorly managed conflicts can slow progress and harm team morale. However, effective conflict resolution can strengthen relationships, enhance problem-solving and improve team performance. Addressing conflicts promptly and effectively keeps the team focused and productive, turning potential issues into opportunities for growth and improvement.

Conflicts are natural and inevitable in any team, especially in high-pressure environments like engineering. The key is not to avoid conflicts but to handle them in a way that leads to positive outcomes. Effective conflict resolution can transform disagreements into opportunities for learning and growth, fostering a more resilient and innovative team.

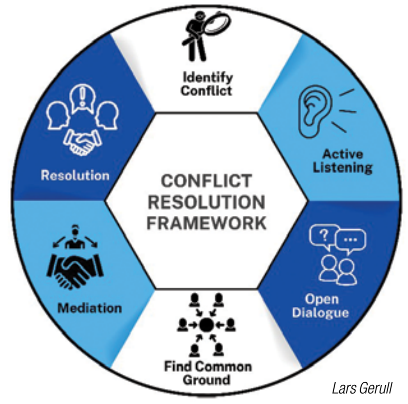


**FIGURE 2. Preventing conflicts from escalating by addressing them as soon as they arise is crucial**

***Common sources of conflict.*** Understanding the root causes of conflict helps in addressing them effectively. Common sources include disputes over resource allocation, differences in priorities and objectives among team members, communication breakdowns and individual differences in work styles and personalities. Identifying these sources early on allows for proactive management and resolution.

***Resource allocation.*** Conflicts often arise over the distribution of resources, such as time, budget and personnel. When team members feel that resources are not allocated fairly or adequately, tensions can build. Clear and transparent decision-making processes can help mitigate these conflicts by ensuring that everyone understands how and why resources are allocated.

***Divergent goals.*** Differences in priorities and objectives among team members can lead to conflicts. For example, one team member might prioritize meeting a deadline, while another might prioritize maintaining high quality. Aligning team goals and ensuring that everyone understands and buys into the overall project objectives can help reduce these conflicts.

***Communication breakdowns.*** Misunderstandings and lack of information sharing are common sources of conflict. When team members are not kept in the loop or when information is miscommunicated, it can lead

to frustration and disputes. Establishing clear communication channels and ensuring that information is shared openly and accurately can help prevent these issues.

***Personality clashes.*** Individual differences in work styles and personalities can lead to conflicts. Some team members might prefer a more structured approach, while others might thrive in a more flexible environment. Recognizing and respecting these differences, and finding ways to accommodate diverse work styles, can help reduce personality-related conflicts.

## Techniques to resolve conflicts

Preventing conflicts from escalating by addressing them as soon as they arise is crucial. An open-door policy encourages team members to voice their concerns promptly. Regular check-ins, like frequent one-on-one meetings, provide an opportunity to discuss any potential issues before they become major problems.

Addressing issues early involves being proactive and attentive to potential conflicts. Leaders should be vigilant for signs of tension and take steps to address them before they escalate. This might involve facilitating discussions, offering mediation, or providing support to team members who are struggling (Figure 2).

***Practice active listening.*** Ensuring that all parties feel heard and understood is key to effective conflict resolution. Reflective listening, where you paraphrase what the other person has said, demonstrates understanding and empathy. Acknowledging the emotions and perspectives of all parties fosters a collaborative approach to resolving conflicts.

Active listening involves more than just hearing what someone says; it requires fully engaging with their message and responding thoughtfully. This means avoiding interruptions, maintaining eye contact and asking clarifying questions. By demonstrating that you genuinely care about understanding their perspective, you can build trust and facilitate a more productive dialog.

***Find common ground.*** Focusing on shared goals and interests helps find mutually acceptable solutions. Collaborative problem-solving involves working together to identify solutions that meet the needs of all parties. Compromise, where team members are willing to give and take, is often necessary to reach an agreement that everyone can accept.

Finding common ground involves identifying the underlying interests and values that team members share. By focusing on these shared aspects, you can shift the conversation from positions of conflict to areas of agreement. This creates a foundation for finding solutions that benefit everyone involved.

***Use mediation.*** In cases where conflicts cannot be resolved internally, consider bringing in a neutral third party. Internal mediators, such as team leaders or human resource professionals trained in conflict resolution, can provide an impartial perspective. External mediators, who specialize in resolving workplace conflicts, can also facilitate a fair and effective resolution process.

Mediation involves bringing in a neutral party to help facilitate discussions and find solutions. Mediators are trained to manage conflicts impartially and can help ensure that all parties are heard and that the resolution process is fair. This can be particularly useful in complex or highly charged conflicts where internal efforts have not been successful.

## Building a collaborative team

Promoting a sense of unity and collaboration within the team enhances overall performance. Team-building activities that encourage teamwork and bonding help create a positive team culture. Establishing clear, common objectives that the entire team works towards fosters a sense of shared purpose and motivation.

***Foster team cohesion.*** Team cohesion involves creating a sense of belonging and mutual support among team members. This can be achieved through activities that build trust and collaboration, such as team-building exercises, social events, and collaborative projects. Encouraging a sense of shared purpose and collective achievement helps strengthen team bonds and improve overall performance.

***Encourage continuous learning.*** Supporting the ongoing development of communication and conflict resolution skills is essential. Training programs, such as workshops and training sessions, provide valuable knowledge and techniques for effective communication and conflict resolution. Mentorship programs, where team members are paired with mentors, offer guidance and support in developing these critical skills.

Continuous learning involves providing opportunities for team members to develop their skills and knowledge. This can include formal training programs, informal learning opportunities and access to resources, such as books, articles, and online courses. Encouraging a culture of continuous improvement helps ensure that team members are always growing and evolving.

***Implement feedback mechanisms.*** Regular feedback helps in continuous improvement. Performance reviews provide opportunities to discuss individual performance and areas for growth. Feedback loops, where team members regularly provide and receive feedback, create a culture of continuous learning and development.

Implementing feedback mechanisms involves creating structured opportunities for feedback to be given and received. This can include regular performance reviews, 360-degree feedback processes and informal check-ins. By fostering a culture of open and constructive feedback, you can help team members grow and develop, and ensure that issues are addressed promptly. ■

*Edited by Dorothy Lozowski*

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**Lars Gerull** is a dedicated life and performance coach specializing in supporting engineers (Email: lars.gerull@yahoo.de). With a deep understanding of the unique challenges engineers face, Gerull addresses issues such as imposter syndrome, burnout, communication hurdles, fear of speaking up and achieving work-life balance. He is passionate about helping engineers unlock their full potential, fostering self-confidence, and improving communication and conflict resolution skills. By providing tailored coaching, Gerull guides engineers toward a fulfilling career and personal life, ensuring they tackle projects with confidence and maintain a healthy balance. He holds an Associate Certified Coach (ACC) certification from the International Coaching Federation (ICF) and an M.S. degree in mechanical engineering from the Cologne University of Applied Sciences.

# Improve Ethylene Production Margins with Digitalization

Digitalization can help ethylene producers to flexibly respond to economic uncertainties and assess available options based on their existing infrastructure and priorities

**Ana Khanlari**
Aspen Technology Inc.

Post-pandemic, olefin and polyolefin producers have been faced with regional and global economic headwinds. Inflation, energy security, rising cost of energy and feedstock, regional conflicts and destocking have impacted their market. To respond to market uncertainties, the industry has worked effectively to close margin gaps through improving operational performance, lowering energy use, and increasing agility to respond to fluctuations requiring rate cuts.

On the environmental front, many ethylene producers have committed to curb emissions by 2030 and 2050 milestones. Such avenues for decarbonization include large-scale electrically heated steam cracker furnaces, such as the one currently under construction at BASF's Ludwigshafen Verbund site in Germany.

Circularity via the mechanical and chemical recycling of waste plastics is another priority for the industry. Renewable plastics (derived from bio-based feedstock or recycled pyrolysis gas) have a lower carbon footprint than ethylene produced in the traditional steam-cracking process. Even though in the short term, the demand for virgin feedstock may not change, in the long-term, product circularity will lower the need for traditional fossil-based feedstock.


**FIGURE 1.** Manufacturing sites are increasingly turning to digital technologies to aid in their training regimens around energy management, plant safety and startups and shutdowns

Digitalization has become integral in ethylene producers' business strategy. Digitalization improves plant performance, efficiency, reliability, safety and product margins, while also playing a key role in developing new technologies for sustainability initiatives. Designing new processes for chemical recycling of plastics, incorporating bio-based and recycled feedstocks, and integrating renewable energy sources are just a few examples. Digital technologies are also necessary for operator training to improve plant safety and expedite planned shutdowns and startups (Figure 1). Leveraging digital solutions, new sustainability project trade-offs can be evaluated, and risks minimized. As the ethylene production landscape is evolving to meet the growing demand, digitalization helps producers balance growth and sustainability.

## Digital solution framework

When it comes to production digitalization, there is a broad spectrum of applications that can improve key performance indicators (KPIs). However, this vast range of solutions can be categorized into three main groups — those contributing to energy efficiency and emissions reduction; those contributing to improving production performance; and those accelerating overall sustainability. In the following sections, only one or two use cases per segment are discussed. Table 1 provides a framework for the applicability and impact of some of the tools and use cases.

**TABLE 1. DIGITAL SOLUTIONS FRAMEWORK FOR ETHYLENE PRODUCTION**

| Improving energy efficiency and emissions management | | |
|---|---|---|
| **Tool** | **Applicability** | **Impact** |
| Digital planning and scheduling tools | Planning, feedstock selection | Minimizing energy use and emissions, boosting throughput, increasing margins |
| Advanced process control (APC) and dynamic optimization tools | Cracking furnaces, light-ends fractionation, compression train | Minimizing energy use and emissions, reducing flaring, reducing cost, increasing throughput |
| Multivariate analytical tools | Cracking furnaces, steam turbines, compressors | Minimizing energy use and emissions, reducing flaring, reducing cost, increasing throughput |
| **Improving production performance** | | |
| **Tool** | **Applicability** | **Impact** |
| Digital twins and real-time optimization | Entire operation | Maximizing productivity, minimizing energy use, reducing flaring |

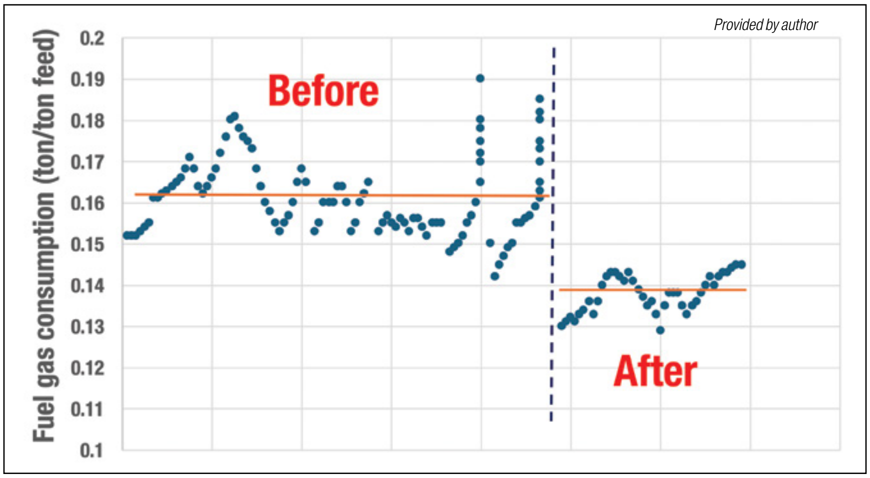


**FIGURE 2. Cracker fuel gas usage is compared before and after the new APC implementation. The crackers on average saved 5% fuel gas with the new APC**

## Energy efficiency and emissions

There are many digital tools available to help plants optimize energy efficiency and reduce emissions production. A few categories are described in the following sections.

***Digital planning and scheduling tools.*** Ethylene producers use digital planning and scheduling (P&S) tools to determine optimal combinations of feedstock, cracking severity and furnace lineups. P&S tools enable them to achieve higher margins while lowering energy use and responding to market opportunities. For multi-site operators, choosing the correct combination of feedstock at each site, production rates and determining marginal ethylene production allocations can maximize gains. These plans are robust and flexible and have lower execution risks. Modern P&S tools enabled with artificial intelligence (AI) and machine learning (ML) capabilities can be trained based on historical data to accelerate schedule creation and initialize optimization. AI-powered interactive advisors can also pro-actively advise planners based on operational constraints.

P&S tools can be integrated with advanced process control and dynamic optimization to provide unique capabilities to operate plants profitably while enabling quick responses to changes in feedstock and product markets. As an example, when an ethylene producer located in the U.S. Gulf Coast region had to cut rates due to an impending hurricane, they minimized lost opportunity by running the optimal feedstock during the rate-cut period. Another producer leveraged production planning optimization to select the optimal feedstock when faced with reliability problems on one of their furnaces, therefore minimizing lost opportunity.

With growing environmental priorities to mitigate emissions and improve energy efficiency, planning and scheduling tools play an additional role in reducing carbon footprints. In a recent study, a major Middle Eastern ethylene producer has used a multi-plant planning model to explore the operational levers available at plant sites to reduce the $CO_2$ footprint of its network of crackers. The study showed that it is possible to decrease cracker $CO_2$ emissions significantly (around 3–5%) by using common operational degrees of freedom without incurring capital expenditures and with minimal impact on olefins production and operating margin. The study explored specific plant economics, operational constraints and flexibility of each plant to achieve an optimum $CO_2$ emissions reduction.

***Advanced process control and dynamic optimization tools.*** Advanced process control (APC) tools have been essential parts of operations for decades. In difficult markets, asset owners direct their investments from larger capital investments and new builds to optimizing and improving productivity, efficiency, sustainability and safety of their existing facilities. APC is one of the strongest tools to achieve economic, safety and sustainability goals with minimal upfront investments. Modern APC tools have expanded capabilities to fit into a wider range of operating conditions. They are self-tuning (adaptive) and self-calibrating thanks to deep learning and AI-embedded functionalities, easier to use and cost less to implement and maintain. While economic objective functions of APC enable producers to run operations to the best of their interest, less experienced engineers can benefit from less complex and AI-guided APC features to run the operation.

In an ethylene plant, APC can be used for a variety of functions. Closing the gap between planning/scheduling and operation, increased agility, following aggressive plans, reducing margin leakage, reducing flaring and $CO_2$ emissions and finally setting the stage for greater autonomy are some of these benefits. For example, when it comes to energy efficiency, a modern APC can model process parameters to execute energy-efficient control actions, update models online with non-disruptive background testing and stabilize processes by minimizing impact of disturbances and process fluctuations on energy use.

Reducing cracking furnaces' fuel use and emissions is an excellent APC use case. Cracking furnaces are the most energy-intensive components of an ethylene plant. A reduction in furnace fuel use by a few percentage points translates to millions of dollars in annual savings, while cutting back on large amounts of $CO_2$ emissions. In a 2019 study, A major Latin American ethylene producer revamped their APC controller in one of their cracking furnaces based on a new control strategy leveraging adaptive control tools. They were able to significantly curb fuel

**TABLE 2. CRACKED-GAS COMPRESSOR SUCTION PRESSURE BEFORE AND AFTER APC IMPLEMENTATION**

| CGC suction pressure | Average ($kg/cm^2$) | Standard deviation |
|---|---|---|
| Pre-APC | 0.52 | 0.043 |
| Post-APC | 0.46 | 0.06 |

usage (Figure 2), leading to $1.15 million in savings per year. Later, the model was expanded to another five crackers.

Cracked gas compressors (CGCs) can also benefit from APC. An estimate of this benefit is presented in Table 2, based on the reduction in suction pressure. A reduction of 0.1 kg/cm$^2$ in suction pressure results in 0.1% increase in ethylene yield, equivalent to about 2 ton/d more of ethylene production.

An olefin plant optimization happens in multiple layers and at different time scales. The planning and scheduling layer, as mentioned earlier, focuses on optimizing the feedstock selection, inventory and furnace swaps monthly or weekly. On the other hand, the APC layer focuses on optimizing feed rate and energy, and meeting product quality on a minute-by-minute basis. In between the planning and APC layers is the middle layer of optimization. It typically involves optimizing feed allocation to the different furnaces, severity/conversion optimization, steam-ratio optimization and suction-pressure optimization performed at the same frequency as the APC layer. Integrating all three layers creates a "unified" platform which streamlines multi-user workflows. While running the plant to its limits, a unified platform can reduce margin leakage by tracking plan execution in real-time. Figure 3 represents KPIs and optimization layers in olefins production.

***Multivariate analysis.*** Multivariate analytical tools for optimization involve data-driven models that provide quick, actionable insights from historical data. Multivariate analysis tools can combine historical and planning data to identify variables with the greatest impact on deviations (for example, energy consumption or product quality). Identifying these variables enables plant engineers and operators to take the necessary actions to adjust operations.

One use case for multivariate analysis is analyzing cracking furnace energy use. In one study, the influence of gas distribution between the side wall and the bottom burners of the furnace was evaluated. Similarly, the best relationship between feed rate and fuel gas consumption was mapped. A range of factors, such as ambient conditions, sensor conditions, feedstock and the specific products can potentially result in operating levels outside of the optimal ranges. In the above example, around 50 to 70 kg/h of fuel gas were saved after implementing the study conclusions.

Improving steam-turbine efficiency is another use case for multivariate analysis. CGCs are large consumers of energy and improving their efficiency lowers steam use and energy cost. However, turbine operation is typically complicated and depends on many factors, such as gas composition, ambient conditions, upstream and downstream operations, performance curves and control targets. With constantly changing demand patterns and non-linear relationships, traditional techniques for calculating efficiency seldom reflect the real world. In a recent study, a global petrochemical company used multivariate analysis to create a single model around turbine and CGC operation, capturing dynamic process behavior and identified factors contributing to efficiency loss. By adjusting these factors, the producer managed to save 5% on turbine steam consumption.

## Production performance

Digital twins and real-time optimization are two tools that engineers can turn to when looking to improve production performance. Digital twins are widely used in industry to provide a digital representation of physical assets and their operations. If the use case is general evaluation and reporting, then an offline steady-state model can be sufficient. However, digital twins can become extremely powerful tools when they receive process measurements directly from the distributed control system (DCS) or plant historian and use the data to optimize the plant and make recommendations for change in real-time (open loop).

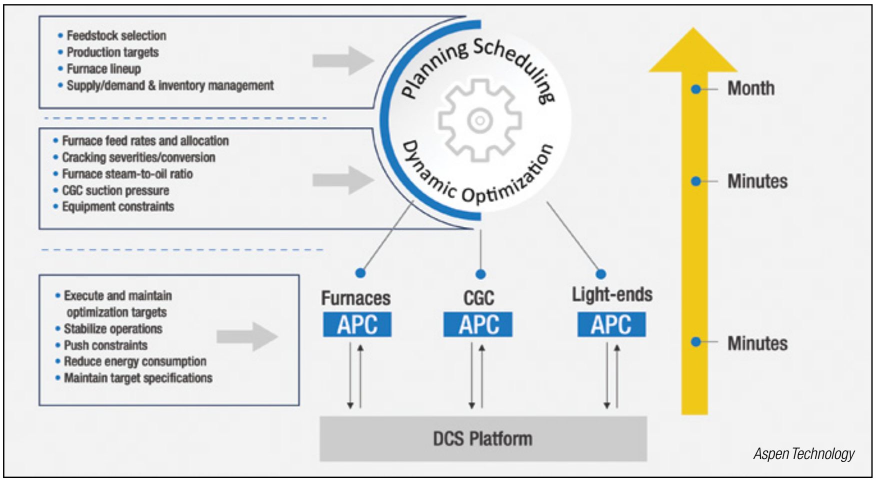


**FIGURE 3. KPIs and optimization layers for the operation are shown. APC and dynamic optimization layers respond to minute-by-minute changes, while planning and scheduling (P&S) has a longer-term outlook**

Online digital twins are extremely useful in olefin plants due to the complexities of the process units and processed feedstocks. Changing feed slate, product profitability and pricing, considerations of energy use, and furnace swaps, among other factors, make real-time monitoring and optimization a necessity. Online optimization can increase the yields of more valuable products, reduce energy consumption per ton of feed or product, push a plant closer to multiple true constraints and increase throughput while evaluating non-linear trade-offs like furnace yields versus refrigeration or distillation.

A major ethylene producer located in the U.S. Gulf Coast region has been using online digital twins for more than 15 years to make trade-offs at the unit level and to maximize gross margins. The site has been able to leverage the tool to improve yield. For instance, when a compressor discharge flow did not match the online model, it led to the discovery of a minimal flow leakage. Fixing the leakage increased the production rate by 1.1%.

## Accelerating sustainability

Many ethylene producers have set sustainability milestones along their decarbonization journey for the coming decades through 2050. Improving energy efficiency and lowering emissions through optimizing operations perhaps has the highest and most immediate impact. However, to truly reshape the industry, many producers are evaluating a diverse range of new technologies.

Leveraging bio-based or recycled feedstocks to produce ethylene is perhaps the next logical step to decarbonize ethylene production. It is estimated that bio-based ethylene production (derived from bio-ethanol) can lower up to 40% of greenhouse-gas emissions associated with ethylene production [*1*]. Chemical upcycling of plastic waste or using sustainable lignocellulosic biomass to produce bio-ethylene are two effective and challenging pathways to reduce production emissions. Digital solutions are fundamental to design, de-risk, scale and understand the technical and economic trade-offs of these processes. Additionally, in markets requiring circular and low-carbon-footprint products, an accurate mass balance of the attributed renewable feedstock is essential. This accurate balance enables producers to obtain certifications, such as REDcert2 or ISCC Plus, for the renewable feedstock used. Digital accounting and reconciliation tools here enable accurate calculations and reporting.

Based on an International Energy Agency estimate, solar, wind and energy efficiency could deliver around half of emissions reduction to 2030 [*2*]. This estimate highlights the power of electrification in energy intensive assets. However, incorporating distributed and intermittent energy sources (wind, solar, geothermal, hydro) requires an advanced distributed-energy resource-management system (DERMS). Digital-grid management solutions ensure sustainability, reliability and resiliency amidst increasingly dynamic supply and demand situations for ethylene producers.

Carbon capture and utilization (CCU) is another way that leading producers can pursue lower carbon emissions. Designing a new steam cracker with built-in capture facilities or retrofitting an existing ethylene plant to add a CCU extension are only possible through digital engineering and economic evaluation tools. Digital solutions help producers with making strategic or detailed decisions like identifying a $CO_2$ destination or determining the required utilities. Technology licensors are leveraging digital engineering to develop $CO_2$-capture facilities to make methanol or green ethylene to further curb emissions.

The global landscape of ethylene production is changing. Flexibility in production and agility to respond to economic uncertainties while responding to consumers' growing needs require new levels of operational excellence. In addition, decarbonization of the chemical industry requires new technologies that don't currently exist at the scales required. Digital solutions provide unique opportunities for the chemical industry to accomplish productivity and sustainability goals for the coming decades. ■

*Edited by Mary Page Bailey*

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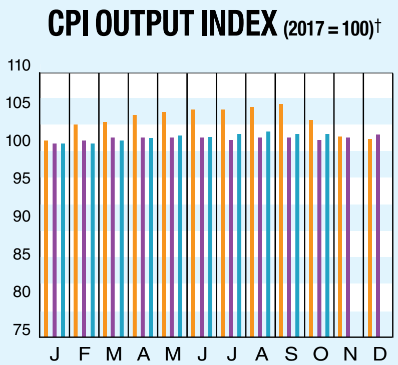
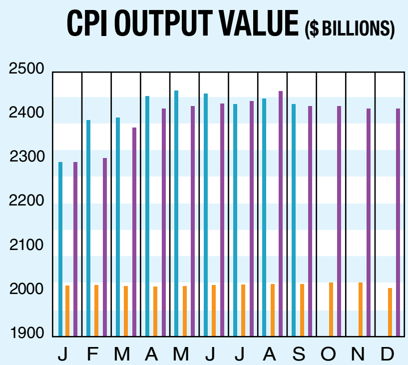
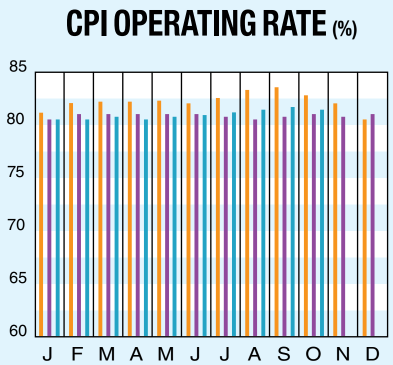
| CURRENT BUSINESS INDICATORS | LATEST | PREVIOUS | | YEAR AGO |
|---|---|---|---|---|
| CPI output index (2017 = 100) | Oct. '24 = 100.7 | Sept. '24 = 100.7 | Aug. '24 = 100.7 | Oct. '23 = 99.7 |
| CPI value of output, $ billions | Sept. '24 = 2,400.2 | Aug. '24 = 2,409.9 | Jul. '24 = 2,433.4 | Sept. '23 = 2,463.8 |
| CPI operating rate, % | Oct. '24 = 77.1 | Sept. '24 = 77.2 | Aug. '24 = 77.2 | Oct. '23 = 77.8 |
| Producer prices, industrial chemicals (1982 = 100) | Oct. '24 = 310.5 | Sept. '24 = 307.4 | Aug. '24 = 311.2 | Oct. '23 = 315.7 |
| Industrial Production in Manufacturing (2017 =100)* | Oct. '24 = 98.5 | Sept. '24 = 99.0 | Aug. '24 = 99.4 | Oct. '23 = 98.9 |
| Hourly earnings index, chemical & allied products (1992 = 100) | Sept. '24 = 235.0 | Aug. '24 = 230.0 | Jul. '24 = 229.1 | Sept. '23 = 227.4 |
| Productivity index, chemicals & allied products (1992 = 100) | Oct. '24 = 94.2 | Sept. '24 = 94.3 | Aug. '24 = 95.6 | Oct. '23 = 93.1 |

**2022** **2023** **2024**




*Due to discontinuance, the Index of Industrial Activity has been replaced by the Industrial Production in Manufacturing index from the U.S. Federal Reserve Board.
†For the current month's CPI output index values, the base year was changed from 2012 to 2017
Current business indicators provided by S&P Global Market Intelligence, New York, N.Y.